NRL Report 5885

A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS

H. G. Norment

Diffraction Branch
Optics Division

April 29, 1963

U. S. NAVAL RESEARCH LABORATORY
Washington, D.C.

CONTENTS

PREFACE

This report contains descriptions and operating instructions for a collection of general utility programs applicable to various phases of crystal structure analysis with computers. All coding is done in FORTRAN II language for 32K core IBM 704 and 7090 machines; the FORTRAN-language programs are completely listed in the Appendix.

The data input to many of the programs has been designed to be compatible with the output of the automatic data reduction program XRDDR (H.G. Norment, "An X-Ray Diffraction Data Reduction Program for the IBM 704 and 7090," NRL Report 5739, Feb. 1962).

Where data input from special tape is required, the logical tape numbers are assigned symbolic designations near the beginnings of the FORTRAN programs. Thus, if it is required that these tape numbers be changed, it is sufficient to change only the one FORTRAN statement card and then recompile.

In the form presented in this report, the programs are written for use with the IBM 7090 IB Monitor system.

PROBLEM STATUS

This is a final report on one phase of the problem; work on other phases continues.

AUTHORIZATION

NRL Problem C07-03
Project RR 001-02-43-4805

Manuscript submitted November 21, 1962.

A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS

1. UNIT CELL PARAMETERS AND ERRORS BY LEAST SQUARES

1.1 Purpose

Given a set of reflection data consisting of Miller indices and $\sin\theta$ or $\sin\theta/\lambda$ values, compute the least-squares reciprocal and real-space unit cell parameters and uncertainties for any crystal system.

1.2 Input

The data input is taken from cards immediately following the program deck. It consists of one control card and a deck of reflection cards.

A. Control Card:

columns	1-2	3-4	5-12	13-72
data	N1	LIST	YAM	Hollerith information
formats	I2	I2	E8.5	10A6

1. N1 specifies the crystal as follows:

Crystal System	N1
triclinic	1
monoclinic*	2
orthorhombic	3
tetragonal	4
hexagonal	5
cubic	6

2. If LIST = 0 or blank, the complete reflection data with observed and calculated $[(\sin\theta)/\lambda]^2$ are printed out. If LIST $\neq$ 0, only the cell parameter and errors are printed.

3. YAM is the wavelength of x radiation used, or else YAM is 0. If YAM = 0 or blank, the program assumes that $(\sin\theta)/\lambda$ values have been loaded. If YAM = λ, the program assumes that $\sin\theta$ values have been loaded.

B. Reflection Card:

columns	1-4	5-8	9-12	13-22	23-32
data	h	k	ℓ	S	W
formats	I4	I4	I4	E10.5	E10.5

1. h, k, ℓ are the Miller indices

2. S is either $\sin\theta$ or $(\sin\theta)/\lambda$ (see above)

3. W is a least-squares weighting factor. If W is not punched, the program assumes W = $(\sin\theta)/\lambda$.

*It is always assumed by the program that c is the unique axis; thus the first setting is used for the monoclinic system.

The reflection card deck is terminated with a blank card.

A second calculation may follow. The reflection deck of the last calculation is terminated with two blank cards.

1.3 Method of Calculation

Let $S^2 = 4(\sin^2\theta)/\lambda^2$

$H_{ij} = h_i h_j$, i, j = 1,2,3

$g^{ij} = a^i a^j$, i, j = 1,2,3

where h_i and a^i are respectively a Miller index and a reciprocal cell edge vector.

Then

$$S^2 = H_{ij}\, g^{ij}$$

where the repetition of a subscript as a superscript in the same term of an expression denotes summation over that index.

The least squares criterion requires that

$$F = \left[W\left(H_{ij}\, g^{ij} - S^2\right)^2\right] = \text{minimum},$$

whence

$$1/2\, \frac{\partial F}{\partial g^{nm}} = \left[W\left(H_{ij}\, g^{ij} - S^2\right) H_{nm}\right] = 0,$$

or

$$\left[W H_{nm} H_{ij}\right] g^{ij} = \left[W S^2 H_{nm}\right],\ n,m,i,j = 1,2,3,$$

where the brackets denote summation over all experimental observations, and W is a weighting factor, different in general for each observation.

After collecting terms, this becomes

$$(2 - \delta_{nm})(2 - \delta_{ij})\left[W H_{nm} H_{ij}\right] g^{ij} = (2 - \delta_{nm})\left[W S^2 H_{nm}\right]$$

where n,m,i, j = 1,2,3; m ≥ n; j ≥ i; and δ_{ij} is the Kroneker delta. In matrix notation this becomes

$$\left(h_{(nm)(ij)}\right) \cdot \left(G_{(nm)}\right) = \left(D_{(nm)}\right)$$

where

$$h_{(nm)(ij)} = (2 - \delta_{nm})(2 - \delta_{ij})\left[W H_{nm} H_{ij}\right]$$

$$G_{(nm)} = g^{nm}$$

$$D_{(nm)} = (2 - \delta_{nm})\left[W S^2 H_{nm}\right].$$

The $G_{(nm)}$ are found by the usual matrix methods. The variances likewise are found by the usual methods, i.e.,

$$\sigma^2 G_{(nm)} = \frac{F}{|h|} \cdot \frac{h^{(nm)(nm)}}{k - \ell}$$

where $h^{(nm)(nm)}$ is the cofactor of $h_{(nm)(nm)}$ element of $|h|$, k is the number of terms in the bracket summation, and ℓ is the order of $|h|$.

The uncertainties in the unit cell parameters and volume are then found by error propagation methods. The equations are quite messy and will not be reproduced here.

1.4 Output

The output is self explanatory. It consists of the reciprocal cell parameters, the real cell parameters with uncertainties, the real cell volume with uncertainty, and, if desired, the observed and calculated S values are listed for each reflection.

1.5 Limitations

No more than 150 observations may be used.

1.6 Special Subroutines Called

In addition to the executive program, the following special subroutines are used:

a. PARAM
b. ERRPRM
c. ERRREL
d. OUTPRM.

Other nonlibrary programs used are:

e. RECIP
f. ARCSIN
g. Modified versions of RW MATS and RW DET (SHARE distn. no. 635).

1.7 Special Tape Requirements

None

2. QUASI NORMALIZATION OF STRUCTURE FACTORS

2.1 Purpose

Prepare a BCD tape containing h,k,ℓ, and ε^2-1, similar to the one written by XRDDR, using for input the h,k,ℓ, F^2 tape written by XRDDR in the Busing least-squares program format (1).

2.2 Input

The input consists of a card input, which is loaded following the program deck, and a tape input, which usually will consist of the data tape output from SUBROUTINE OUTPUT of XRDDR. The tape input is from logical tape 16.

A. Control Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	NOIB	NASP	NF	BT1	EX	LIB
formats	I10	I10	I10	E10.4	E10.4	I10

1. NOIB is the number of reflection records on logical tape 16.

2. NASP is the number of different atomic species in the crystal.

3. NF is the number of files on the input tape to be spaced over. This allows input to be taken from a library tape.

4. BT1 is the modified Wilson equation temperature factor B (as taken directly from the output of XRDDR).

5. EX is the exponent in the modified Wilson equation (labeled X in the output of XRDDR).

6. LIB is 1 if a library tape is used as input. It is blank otherwise. (It is assumed that the first record of a library tape is an identification record.)

Atomic Scattering Factor Cards:

columns	1-8	9-16	17-24	25-32	33-40	41-44
data	AS	AS1	BS	BS1	CS	AN
formats	F8.4	F8.4	F8.4	F8.4	F8.4	F4.0

The quantities AS, AS1, BS, BS1 and CS are the parameters A, a, B, b, and C defined and listed by Forsyth and Wells for calculation of atomic scattering factors (3). AN is the number of atoms of the atomic species in the unit cell. There is one card for every different atomic species in the crystal. The deck consists of one control card followed by NASP atomic scattering factor cards.

B. Reflection Data Tape:

columns	1-9	10-18	19-27	28-36	37-54	55-63
data	h	k	ℓ	F^2	blank	$(\sin\theta)/\lambda$
formats	F9.2	F9.2	F9.2	F9.2	18X	F9.6

2.3 Method of Calculation

F^2 values are converted to ϱ^2 values according to the following equation

$$\varrho^2 = F^2\left(\exp\left[B\left(\frac{\sin}{\lambda}\right)^2\right]\right)\Big/\left(\sum^{N} f^2\right).$$

The reflections are read from the input tape and processed in groups of 500 (or less for the last group). Thus, any number of reflections may be processed in one computer run.

2.4 Output

Logical tape 15 is rewound at the beginning of the calculation. Output is BCD on tape 15. The program writes an END FILE on 15 and rewinds it when the calculation is finished.

columns	1-4	5-8	9-12	13-32
data	h	k	ℓ	ξ^2-1
formats	I4	I4	I4	F20.5

2.5 Limitations

There can be no more than twenty different atomic species in the crystal.

2.6 Special Subroutines Called

A FAP coded subroutine FLSKPD is called which forward-spaces tape 16 the number of files specified by NF (see control card).

2.7 Special Tape Requirements

Logical tape 16 is used for BCD reflection input.

3. RATIONAL DEPENDENCE*

3.1 Purpose

To determine the extent of rational dependence, as defined by Hauptman and Karle (4), in a crystal structure using the normalized structure factor magnitudes.

3.2 Input

The input consists of a card input, which is loaded following the program deck, and a tape input, which usually will consist of the data tape output from program SF NORM of XRDDR. The tape input is from logical tape 12.

A. Card Input

There are two types of cards in the card input.

a. 72 columns of Hollerith characters (these characters are used to title the output).

b. Control Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60	61-70
data	NA	NINT	NFIN	MINN	AN	SDMIN	JPUT
formats	I10	I10	I10	I10	E10.4	E10.4	I10

1. NA is 1 for noncentrosymmetric crystals; it is 0 or blank for centrosymmetric crystals.
2. NINT is the initial modulas.

*After Block and Yannoni, National Bureau of Standard (unpublished).

3. NFIN is the final modulas.

4. MINN is the minimum number of reflections considered significant in a subset showing rational dependence effects. Results will not be output for subsets of reflections with fewer than MINN members.

5. AN is the minimum number of standard deviations which is considered a significant difference between the subset average and overall average of E^2.

6. SDMIN is the smallest deviation between the subset average and the overall average of E^2, where the deviation is considered to significantly show the presence of rational dependence effects.

7. JPUT is not 0 when complete listings of reflections are desired for each subset for which evidence of rational dependence has been found. JPUT is 0 when the reflection listings are not desired.

Additional control cards may follow if additional calculations are desired. The card deck is terminated with a blank card.

B. Tape Input.

This tape may be tape number 5 or 7 from program SF NORM of XRDDR:

1. The first record on the tape consists of the number of reflection records on the tape (format I7).

2. Reflection records:

columns	1-4	5-8	9-12	10-32
data	h	k	ℓ	E^2-1
formats	I4	I4	I4	F20.5

3.3 Method of Calculation

A FORTRAN source program written by Block and Yannoni was obtained from Dr. Block of the National Bureau of Standards. The program has been modified with respect to reflection input; certain redundancies in the selection of subsets have been eliminated; a provision for specifying the minimum significant number of reflections in the subsets has been added; the criterion for accepting as significant a deviation of average E^2 from the overall value has been operationally improved by making it independent of the numbers of reflections in the subsets; and, finally, the output has been vastly expanded and improved. Otherwise the calculations are done essentially as coded by Block and Yannoni.

All reflections in a subset satisfy the relation

$$ah + bk + c\ell \equiv n \pmod{m}$$

where m is a positive integer limited (by the program) to a maximum value of 14; a, b, and c may have integral values ranging from -13 to +14, depending upon the value of m.

If the value of average E^2 for a subset differs significantly from the average over all observed E^2, then rational dependence is said to exist in the crystal structure.

The program automatically checks all possible subsets for rational dependence effects for all moduli (i.e., all m) between the limits specified on the control card.

3.4 Output

The output consists of three parts A, B, and C. A and B are always obtained, and C is or is not obtained at the option of the program user.

A. This is a leading one-page printout consisting of the control information, overall average E^2, and the total number of reflections on the input tape.

B. For each subset for which significant rational dependence effects are found the following is printed: a,b,c,n,m, average E^2, and the number of reflections in the subset.

C. If the control datum JPUT is not zero, data for all reflections in the subset defined by the printout of B above are listed, immediately following the B printout, in the form: h,k,ℓ, E^2-1, and E^2-A, where A is the overall average E^2.

3.5 Limitations

The only limitation in addition to those already mentioned in section 3.3 is that the number of input reflections be less than 5000.

3.6 Special Subroutines Called

A subroutine OUTRAT, especially designed to write output for this program, is called.

3.7 Special Tape Requirements

Logical tape 12 is used for reflection input.

4. SIGMA-2 LISTINGS

4.1 Purpose

For each member of an ordered list of reflections, where the member is defined by the Miller index triple $\vec{h}$ and normalized structure factor magnitude E, the program lists all pairs of reflections $\vec{h}_i$, E_i, and $\vec{h}_j$, E_j from a similar ordered list of reflections which satisfy the relation

$$\vec{h} = \vec{h}_i + \vec{h}_j .$$

A pair of reflections $\vec{h}_i$ and $\vec{h}_j$ is said to be a Σ_2 interaction pair for the reflection $\vec{h}$ if the equation above is satisfied.

4.2 Input

The data input consists of one control card, which is positioned at the end of the program deck, and a list of h and E^2-1, which is read in either from logical tape 11 or from cards. The output tapes from program SF NORM of XRDDR may be used.

A. Control Card:

columns	1-10	11-20	21-30
data	Z	IZ	NOIB
formats	E10.4	I10	I10

1. All reflections for which $E^2-1 < Z$ are rejected from consideration.

2. If IZ = 0 the reflection data are read from logical tape 11. If IZ $\neq$ 0 the reflection data are read from cards.

3. Lists of Σ_2 interaction pairs are tabulated for the NOIB reflections with largest E^2-1 values. If NOIB is negative, lists are prepared for the entire group of reflections for which $E^2-1 \geq Z$ (see method of computation below).

B. Reflection Data.

The reflection data is prefaced with one card (or record) NRT containing the number of reflections to be read. The format is I7.

The reflection records contain the following information:

columns	1-4	5-8	9-12	13-32
data	h	k	ℓ	E^2-1
formats	I4	I4	I4	F20.5

4.3 Method of Calculation

As each reflection is read into the computer it is accepted or rejected on the basis of whether or not the criteria on h,k,ℓ specified in REJVEC (see section 4.5) are satisfied. If the criteria are not satisfied, REJVEC sets $E^2-1 = -10$. Then, the reflection is tested on the basis of the magnitude of E^2-1, and all reflections for which $E^2-1 < Z$ are rejected. (The minimum physically meaningful value of E^2-1 is -1.)

The selected set of reflections is arranged in decreasing order of magnitude of E^2-1. Then lists of Σ_2 interaction pairs are calculated and tabulated for the top NOIB reflections in the selected set. If NOIB has been entered as a negative number, the lists are calculated for every member of the selected set.

4.4 Limitations

The selected set of reflections may not exceed 2400 reflections. There may not be more than 1000 Σ_2 interaction pairs for each $\bar{h}$.

4.5 Special Subroutines Called

a. REJVEC.

This subroutine imposes acceptance criteria on h,k,ℓ of each reflection. The program user may write his own program or use the dummy program already written. The quantities N1, N2, N3, and Q in the calling sequence are h,k,ℓ, and E^2-1.

b. SIGVEC.

A crystal-system-dependent subroutine which selects $\vec{h}_i$ and $\vec{h}_j$ for each $\vec{h}$. If SIGVEC for the triclinic case is used, and the reflection decks are always "blownup" so as to include all symmetry mates of all reflections, then this subroutine becomes noncrystal-system dependent. SIGVEC versions for triclinic, monoclinic, and orthorhombic crystals are available.

c. OUTSIG.

This subroutine prints out the list of $\vec{h}_i$, E_i and $\vec{h}_j$, E_j and the products $E_i E_j E$ for each $\vec{h}$, E.

4.6 Special Tape Requirements

Logical tape 11 is used for reflection input.

5. TRIPLE PRODUCT SUMMATION FOR ORTHORHOMBIC CRYSTALS

5.1 Purpose

These programs (one for centrosymmetric and one for noncentrosymmetric crystals) are designed to calculate the quantity $E_1E_2E_3$, as defined by Hauptman and Karle (5), or the quantity $|E_1E_2E_3| \cos(\phi_1+\phi_2+\phi_3)$, as defined by Karle and Hauptman (6).

5.2 Input

The input consists of a card input, which is loaded following the program deck, and a tape input, which usually will consist of an output tape from program SF NORM of XRDDR.

A. Control Card:

columns	1-10	11-20	21-30	31-40
data	NA	IM	JM	KM
formats	I10	I10	I10	I10

1. NA is the number of atoms (exclusive of hydrogen atoms) in the unit cell.
2. IM is the maximum value of Miller index h.
3. JM is the maximum value of Miller index k.
4. KM is the maximum value of Miller index ℓ.

Triple Product Selection Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	h_1	k_1	ℓ_1	h_2	k_2	ℓ_2
formats	I10	I10	I10	I10	I10	I10

1. h_1, k_1, ℓ_1 are the Miller indices of the reflection with normalized structure factor E_1 (see section 5.1).

2. h_2, k_2, ℓ_2 are the Miller indices of the reflection with normalized structure factor E_2 (see section 5.1).

The deck consists of one control card followed by any number of triple product selection cards. Calculation is terminated by the second blank card read (the first blank card causes calculation of the triple for $\vec{h}_1, \vec{h}_2 = 0$).

B. Reflection Data.

The first record on the reflection data input tape contains the number of reflection records to follow (format I7).

Each reflection record consists of:

columns	1-4	5-8	9-12	13-32
data	h	k	ℓ	E^2-1
formats	I4	I4	I4	F20.5

Tape input is from logical tape 9.

For many problems it may be necessary to recompile the source program in order that the dimension assignments on the triply indexed variable E be changed (see section 5.3).

5.3 Method of Calculation

The program stores each value of $(E^2-1)_{hk\ell}$ as the triply indexed FORTRAN variable $E(h,k,\ell)$. The program then runs through the list of reflections in a triple nest of DO loops in order to select summands.

The orthorhombic symmetry operations on h,k,ℓ are coded into the program.

Since the program uses h,k,ℓ as indices, these quantities always must be positive. The program automatically rejects one- and two-dimensional data. Core size limits the maximum values of h,k,ℓ rather severely. As listed in this report, the program accepts maximum values of h,k,ℓ as large as 30, 10, 30. E is the only dimensioned variable in the programs, and most of the core is available to it; however it will frequently be necessary to recompile.

The only difference between the programs for centrosymmetric and noncentrosymmetric crystals is that for the former, the average is divided by $\overline{NA}^{3/2}/8$, whereas the latter is divided by $\overline{NA}^{3/2}/2$. (Note the third statement following statement number 8 in the FORTRAN listing given in Appendix A.)

Whereas only three-dimensional data are included in the summations, $\vec{h}_1, \vec{h}_2, \vec{h}_3$ need not be three dimensional.

If none of the Miller indices of $\vec{h}_1, \vec{h}_2, \vec{h}_3$ are zero, the program includes the correction term $(E^2_{\vec{h}_1} + E^2_{\vec{h}_2} + E^2_{\vec{h}_3} - 2)/\overline{NA}^{1/2}$ in the results.

5.4 Output

The output for each reflection includes:

a. $\vec{h}_3, \vec{h}_1, \vec{h}_2$
b. the number of terms in the sum.
c. the scaled triple product average without correction term.
d. the scaled triple product average with correction term.
e. the correction term.

5.5 Limitations

See section 5.3.

5.6 Special Subroutines Called

None.

5.7 Special Tape Requirements

Logical tape 9 is used for reflection input.

6. STRUCTURE FACTOR CALCULATION

6.1 Purpose

To provide a convenient means for calculation of structure factors and quasi-normalized structure factors for use during preliminary stages of structure determination. Reflection input is from the E^2-1 or F^2 output tapes of XRDDR. Isotropic temperature factors are used.

6.2 Input

The input may be divided into general and control information, and reflection data.

A. General and Control Information.

The cards in this part are included with the program deck.

1. 72 columns of Hollerith characters (format 12A6). These Hollerith characters are used to title the output.

2. Control Card No. 1:

columns	1-10	11-20	21-30	31-40	41-50	51-60	61-70
data	IC	IE	NR	NF	IP	LIB	LINE
formats	I10	I10	I10	I10	I10	I10	I10

IC = 0 if crystal is centric; IC ≠ 0 if crystal is acentric.

IE = 0 if F^2 reflection data input is used; IE ≠ 0 if E^2-1 reflection data input is used.

NR is the number of input reflections (if E^2-1 reflection data is used, this may be left blank).

NF is the number of files to be spaced over if the reflection data are read from a library tape.

IP = 0: E output mode is specified; IP ≠ 0: F output mode is specified. IP is irrelevant for centric crystals (see section 6.5.B for a description of the modes).

LIB = 0: library tape not used for reflection input; LIB ≠ 0: library tape is used for reflection input.

Line = 0: reflection data is read from logical tape 10; LINE ≠ 0: reflection data is read from cards.

3. Cell Constant Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	a	b	c	α	β	γ
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

$a, b, c, \alpha, \beta, \gamma$ are the real-space unit cell parameters in units of angstroms and degrees.

4. Control Card No. 2:

columns	1-10	11-20	21-30	31-40	31-50
data	BT	XT	SFC	KKT	IOUT
formats	E10.4	E10.4	E10.4	I10	I10

BT and XT are the parameters B and X of the modified Wilson equation as taken from the output of XRDDR (if KKT = 1, these fields may be left blank).

SFC is a scale factor by which all F_0 are to be multiplied to bring them to the proper scale. It is irrelevant if E_0 data are input.

KKT has the value of 0,1, or 2, which serves to select the desired structure factor normalization procedure as follows:

KKT = 0: apply exact normalization procedure to F_c; apply approximate normalization procedure to F_0 or E_0.

KKT = 1: apply exact normalization procedure to F_c; apply exact normalization procedure to F_0 or E_0.

KKT = 2: apply approximate normalization procedure to F_c; apply approximate normalization procedure to F_0 or E_0.

(see section 6.4 for explanations of exact and approximate normalization.)

If IOUT ≠ 0, a BCD output (logical tape 11) will be written (see section 6.6).

5. Scale factor cards.

If IE is 0 (i.e., F_0 reflection data are input), a deck of scale factor cards is input. Each card contains one scale factor (format E10.4). The deck is terminated with a blank card. The scale factors are indexed in the order loaded and are applied according to the procedure given in section 6.2.B under description of SCF.

6. Atomic scattering factor cards.

There is one card for each unique atomic species in the crystal:

columns	1-8	9-16	17-24	25-32	33-40
data	A	a	B	b	C
formats	F8.4	F8.4	F8.4	F8.4	F8.4

A, a, B, b, and C are the parameters used in the Vand, Eiland, Pepinsky approximation equation for calculation of atomic scattering factors as defined by Forsyth and Wells (3,7).

The deck of atomic scattering factor cards is terminated by a blank card.

The loading order of the atomic scattering factor cards is important and must be consistent with the quantities I on the coordinate cards (see section 6.2.A.7).

7. Coordinate cards.

There is one card for each atom in the asymmetric unit:

columns	1-10	11-20	21-30	31-40	41-50
data	X	Y	Z	B	I
formats	E10.4	E10.4	E10.4	E10.4	I10

X,Y, and Z are the fractional atomic coordinates of one atom.*

B is the isotropic temperature factor.

I is an integer which relates the atom to one of the atomic scattering factor cards and thus specifies the atomic type. Each atomic scattering factor card is numbered 1,2,3,... in sequence as it is read into the computer. Thus, if the second scattering factor card to be read is for carbon, then I = 2 on all carbon coordinate cards.

The deck of coordinate cards is terminated with a blank card.

8. Transformation cards.

The atoms in the asymmetric unit are transformed according to the relations given in "International Tables for X-Ray Crystallography," Vol. I, (N.F.M. Henry and K. Lonsdale, Birmingham: Kynoch Press, 1952) so as to fill out the unit cell. There is one card for each transformation.

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	T1	T2	T3	U1	U2	U3
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

*If an atom is at the origin, X,Y,Z should be given the values 1,1,1 instead of 0,0,0.

The transformations are done as follows:

$$X' = T1 + U1 \cdot X$$
$$Y' = T2 + U2 \cdot Y$$
$$Z' = T3 + U3 \cdot Z.$$

Example: Space group $P2_1/c$

Transformations: $\bar{x},\bar{y},\bar{z}$; $x,1/2 - y, 1/2 + z$; $\bar{x}, 1/2 + y, 1/2 - z$.

Transformation cards

T1	T2	T3	U1	U2	U3
.0	.0	.0	-1.	-1.	-1.
.0	.5	.5	1.	-1.	1.
.0	.5	.5	-1.	1.	-1.

The deck of transformation cards is terminated with a blank card.

B. Reflection Data.

The reflection input may be included along with the program deck, following the general and control information cards, or be taken from logical tape 10. It may be taken directly from an XRDDR output tape or from a library tape, each file of which contains the data from an XRDDR input or output tape. In the latter case, the program assumes that each file is prefixed with one identification record.

The program calculates structure factors for each reflection in the reflection input.

If F_0^2 reflection input is used $(\sin\theta)/\lambda$ values may or may not be included (they are automatically included on the XRDDR F^2 output tapes). The format is the same as that used for input to the Busing least-squares program.

If E^2-1 reflection input is used, the first record must consist of the number of reflections to be read (format I7). No provision is made for input of $(\sin\theta)/\lambda$ data.

F^2 reflection data:

columns	1-9	10-18	19-27	28-36	37-45	46-54	55-64
data	h	k	ℓ	F_0	(blank)	SFC	$(\sin\theta)/\lambda$
formats	F9.2	F9.2	F9.2	F9.2	9X	F9.2	F9.6

The quantity SCF is a floating point integer which relates the reflection to one of the scale factors described in section 6.2.A.5 above. The integer corresponds to the loading sequence number of the scale factor (i.e., the first scale factor loaded corresponds to SCF = 1.0, etc.). SCF may be punched on every card. Alternatively, the reflection input may be grouped into sets where all reflections in a set are multiplied by the same scale factor. In this case, it is sufficient to punch SCF in the first card only of each set. This is the same scaling procedure used in the Busing least-squares refinement program; however, in this program, the F_0 values are scaled.

E^2-1 reflection data:

columns	1-4	5-8	9-12	13-32
data	h	k	ℓ	$E_0{}^2$-1
formats	I4	I4	I4	F20.5

If another calculation is to follow, a card with a 1 punched in column 7 follows the last card of the main deck; otherwise, a blank card is last.

6.3 Data Deck

The composition of the data deck is as follows:

a. Hollerith card.
b. control card no. 1.
c. cell constant card.
d. control card no. 2.
e. all scale factor cards (if IE $\neq$ 0, there are no scale factor cards).
f. blank card.
g. all atomic scattering factor cards.
h. blank card.
i. all coordinate cards.
j. blank card.
k. all transformation cards (if any).
l. blank card.
m. reflection cards unless reflection input is from tape.
n. a card with 1 in column 7 or a blank card depending upon whether or not another calculation is to follow.

6.4 Method of Calculation

Structure factors are calculated from the total unit cell contents (rather than from the asymmetric unit contents) using the equations for the triclinic case. Nevertheless, coordinates may be entered for one asymmetric unit only, provided that transformations follow by which the asymmetric unit set is expanded to fill the unit cell. The transformations may be copied directly from the "International Tables for Crystallography," Vol. I (1952). In this way, the program is completely general in its applicability while requiring the most simple type of input.

The quasi normalization of structure factors (and in the case where E^2-1 reflection input is used, the inverse normalization) may be done in either of two ways, designated as exact and approximate normalization.

1. Exact normalization:

$$E^2 = F^2 \Big/ \sum_{i=1}^{n} f_i^2 .$$

2. Approximate normalization:

$$E^2 = \frac{F^2 \exp\left[BT(\sin^2\theta/\lambda^2)^{xT}\right]}{\sum_{i=1}^{N} f_{0,i}^2},$$

where

$$f_i = f_{0,i} \exp\left[-B_i(\sin^2\theta)/\lambda^2\right]$$

and N is the number of atoms in the unit cell.

6.5 Printed Output

A. Centric Crystals.

The output for each reflection is:

a. h,k,ℓ
b. F_0
c. F_c
d. E_0
e. E_c
f. ΔF
g. ΔE.

B. Acentric Crystals.

Either one of two modes of output may be selected:

1. F mode

a. h,k,ℓ
b. E_0, E_c
c. F_0, E_c
d. A_0, B_0
e. A_c, B_c
f. ΔA, ΔB
g. ΔF.

2. E mode

a. h,k,ℓ
b. F_0, F_c
c. E_0, E_c
d. C_0, C_c
e. D_0, D_c } where $|E|^2 = C^2 + D^2$
f. ΔC, ΔD
g. ΔE.

In addition to the reflection output, the program prints $\Sigma|\Delta F|$, $\Sigma|F_0|$, and $R = \Sigma|\Delta F| / \Sigma|F_0|$ both including and excluding unobserved data.

6.6 Tape Output

If IOUT $\neq 0$ the program writes a reflection output tape containing one of the following sets of data for each reflection (format 7F10.4):

a. Centrosymmetric crystals

$$h, k, \ell, F_0, E_0, \Delta F, \Delta E$$

b. Noncentrosymmetric crystals

1. IP = 0:
   $h, k, \ell, C_0, D_0, \Delta C, \Delta D$
2. IP $\neq$ 0:
   $h, k, \ell, A_0, B_0, \Delta A, \Delta B$

where the observed quantities are scaled and given the signs of the corresponding calculated quantities.

6.7 Special Subroutines Called

a. OUTSFC.
   An output routine designed for these calculations only.

b. RECIP.

c. The FAP coded tape utility program written by P. Gum.*

d. INTG.

6.8 Special Tape Requirements

a. Logical 10 is used for reflection input.

b. Logical 11 is used for reflection output.

7. INTERATOMIC DISTANCES AND ANGLES WITH INTERPOLATION FOR PEAK CENTER LOCATION

7.1 Purpose

Given a basic set of atomic or peak coordinates and a set of symmetry transformations on these coordinates, calculate and list all interatomic distances b, where $0.7 \leq b \leq BMX$, and calculate all angles between connected pairs of distances for all possible combinations in any crystal.

---

*Diffraction Branch, Optics Division, NRL.

7.2 Input

The data input is from cards which are loaded immediately following the program deck. The cards are described in loading sequence as follows:

A. 72 columns of Hollerith characters (format 12A6). These Hollerith characters are used to title the output.

B. Cell Constant Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	a	b	c	α	β	γ
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

The quantities $a, b, c, \alpha, \beta, \gamma$ are the real-space unit cell parameters expressed in units of angstroms and degrees.

C. Bond Length Limit Card:

columns	1-10	11-20
data	BMX	AMX
formats	E10.4	E10.4

BMX.

Interatomic distances b for which $0.7 \leqslant b \leqslant$ BMX are considered acceptable and are tabulated for printing.

AMX.

Angles for all pairs of acceptable distances sharing a common atom, for which the distances of both members of the pair are less than or equal to AMX, are tabulated for printing.

[WARNING: When a large number of atoms or peaks are involved and BMX and AMX are both large (i.e., greater than about 3.0A), the number of angles printed can be very large.]

D. Grid Interval Card:

If peak maxima coordinates are to be found by interpolation between grid points of a Fourier calculation result, this card contains the fractional grid increments in the directions of X, Y, and Z.

columns	1-10	11-20	21-30
data	XINC	YINC	ZINC
formats	E10.4	E10.4	E10.4

For example, if the Fourier calculation was done in increments of 1/30, 1/60, and 1/120 along X, Y, and Z, respectively, then

XINC = .03333, YINC = .01666, and ZINC = .008333.

If interpolation is not to be done, this card must be blank.

E. Coordinate Card:

columns	1-10	11-20	21-30
data	X	Y	Z
formats	E10.4	E10.4	E10.4

X, Y, and Z are the fractional coordinates of an atom or peak. There is one card for each atom or peak in the basic (untransformed) set. If interpolation is to be done, each coordinate card is followed by an interpolation card (see section 7.2.F below). If interpolation is not to be done, the interpolation cards are absent from the deck.

The coordinate card deck is terminated by a blank card.

F. Interpolation Card.

Interpolation cards are included in the coordinate deck, one following each coordinate card, if and only if card D is not blank (see section 7.2.D). .2.4).

The fractional coordinates of the grid point closest to a peak maximum in a Fourier calculation result are given on the coordinate card. Relative to this central grid point, designate the Fourier summation value at nearby grid points by P(i, j, k), where i, j, and k have integral values representing the (signed) numbers of grid interval separations of the point from the central one in the directions of X, Y, and Z, respectively.

The interpolation card contains the following:

columns	1-10	11-20	21-30	31-40	41-50	51-60	61-70
data	P(0,0,0)	P(-1,0,0)	P(1,0,0)	P(0,-1,0)	P(0,1,0)	P(0,0,-1)	P(0,0,1)
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

If the user wishes to interpolate some, but not all, points, then values of P(0,0,0) = 100.0 and all other P = 1.0 may be entered for those points that are not to be interpolated.

Note that P(0,0,0) must be the largest P on the card. Also, all P must be greater than zero. Negative or zero P can be accommodated by adding a constant increment to all P such that the results are all positive.

G. Transformation Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	T1	T2	T3	U1	U2	U3
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

There is one transformation card for every symmetry transformation to be applied to the basic set of coordinates. The transformations are applied according to the equations:

$$X^1 = T1 + U1 \cdot X$$

$$Y^1 = T2 + U2 \cdot Y$$

$$Z^1 = T3 + U3 \cdot Z.$$

The transformation card is terminated by a blank card.

7.3 Data Deck

The composition of the data deck is as follows:

a. Hollerith card.
b. cell constant card.
c. bond length limit card.
d. grid interval card, or blank if interpolation is not desired.
e. all coordinate and interpolation cards.
f. blank card.
g. all transformation cards (if any).
h. blank card.

7.4 Method of Calculation

The basic set of coordinates are loaded, interpolated (if desired), and then each transformation is applied to the basic set, generating a transformed set for each transformation. Thus, if there are N atoms in the basic set and there are M transformations, the complete set contains N(M + 1) atoms.

Interatomic distances less than or equal to BMX are tabulated for all pairs of atoms in the basic set and for all distances ($\leq$ BMX) which cross the transformed set boundaries for the complete set.

Atom pairs closer together than 0.7A are listed in a separate output and are rejected from further consideration.

Next, the list of accepted interatomic distances is scanned to find pairs of interatomic distances which share a common atom. Angles for all such pairs of distances are tabulated if both distances are less than or equal to AMX. Logical tape 9 is used for intermediate storage of angles.

Interpolation is done by fitting the seven Fourier grid points closest to the peak maximum to a Gaussian function and then finding the maximum of the function. The corrections, ΔX, ΔY, and ΔZ to be added to X, Y, and Z are found by solving the matrix

$$\begin{pmatrix} \vec{a}\cdot\vec{a} & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{a}\cdot\vec{b} & \vec{b}\cdot\vec{b} & \vec{b}\cdot\vec{c} \\ \vec{a}\cdot\vec{c} & \vec{b}\cdot\vec{c} & \vec{c}\cdot\vec{c} \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix} = \begin{pmatrix} D_x \\ D_y \\ D_z \end{pmatrix}$$

where

$$D_x = \frac{a^2}{2}\left[\log \frac{P(1,0,0)}{P(-1,0,0)}\right] \Big/ \left[\log \frac{P(0,0,0)}{P(1,0,0)} + \log \frac{P(0,0,0)}{P(-1,0,0)}\right],$$

etc.

7.5 Output

In the output, each atom is represented by two integers separated by a hyphen. The first integer specifies the transformation (numbered according to loading order) which has been applied, and the second integer specifies the atom in the basic set (numbered according to loading order) from which it was derived.

The output is in the following order:

a. Atomic coordinates for the complete set.

b. Interatomic distances.

c. Angles.

d. Interatomic distances less than 0.7A.

7.6 Limitations

a. The complete set of atoms or peaks is limited to 500 in number.

b. If more than 2900 acceptable interatomic distances are found, BMX is decremented by 0.25A and the calculation is begun again. This process is repeated until a total of 2900, or less, acceptable distances are found, or until BMX $\leq$ 2.0. In the latter case, distances and angles are calculated for the basic set of atoms only. If more than 2900 acceptable distances are found in the basic set, the calculation is terminated without output of results.

c. No more than 200 distances less than 0.7A can be accommodated.

d. There is no limit on the number of bond angles.

7.7 Special Subroutines Called

a. subroutine INTERP. This subroutine does the interpolation by Gaussian curve fitting.

b. subroutine MATS (SHARE distr. no. 635).

c. soubroutine OUTBND: (distance and angle output).

d. function DOTPRD.

e. function ARCSIN.

7.8 Special Tape Requirements

Logical Tape 9 is used for intermediate storage.

8. LEAST-SQUARES PLANE AND LINE FITTER

8.1 Purpose

This program fits planes and/or lines to sets of points and calculates angles between planes and lines which have been fitted.

8.2 Input

a. 72 columns of Hollerith characters (format 12A6). These Hollerith characters are used to title the output.

b. Unit Cell Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	a	b	c	α	β	γ
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

The quantities $a,b,c,\alpha,\beta,\gamma$ are the real-space unit cell parameters expressed in units of angstroms and degrees.

c. Plane or Line Specification Card:

columns	10-3	4-6	7-12	13-72
data	N	NO	L	Hollerith
formats	I3	I3	I6	10A6

N is the number of points to be fitted.

NO is the plane or line number.

L = 0 or blank if the points are to be fitted to a plane.

L = 1 if the points are to be fitted to a line.

The Hollerith characters in columns 13-72 are used as a page heading for the line or plane in the output.

d. Coordinate Card:

columns	1-10	11-20	21-30	31-40
data	X	Y	Z	W
formats	E10.4	E10.4	E10.4	E10.4

X, Y, and Z are fractional coordinates of a point to be fitted to a line or plane.

W is a least-squares weighing factor. If W is not punched, it is assumed to have a value of one by the program.

e. Angle specification card.

This card specified a plane-plane, line-line, plane-line, or line-plane pair for which the dihedral angle is to be calculated.

columns	1-3	4-6	7-9	10-12
data	NO1	L1	NO2	L2
formats	I3	I3	I3	I3

NO1 is the number of the first plane or line.

LI = 0 or blank if NO1 refers to a plane.

LI = 1 if NO1 refers to a line.

NO2 is the number of the second plane or line.

L2 = 0 or blank if NO2 refers to a plane.

L2 = 1 if NO2 refers to a line.

The plane and line numbers NO are used to identify the different planes and lines both internally and in the output. The numbering may be different from the order of input. No two planes may have the same number, and no two lines may have the same number, but the numbering of lines and planes is independent. The number of any plane or line must not be greater than 50.

8.3 Data Deck

The composition of the data deck is as follows:

a. Hollerith card.

b. unit cell card.

c. plane or line specification card.

d. all coordinate cards for this plane or line (the number of coordinate cards must be the same as the N punched on the preceding plane or line specification card).

e. plane or line specification card.

f. all coordinate cards for this plane or line.

g. additional sets of specification and coordinate cards for as many planes and lines as are to be fitted.

h. blank card.

i. all angle specification cards, if any.

j. blank card.

8.4 Method of Calculation

The method described in detail by Shomaker, Waser, Marsh, and Bergman (8) is used.

The program is written in the fullest generality so as to be able to handle points defined in any three-dimensional coordinate system. However, no provision is made for symmetry transformation of point positions, so all points must be properly transformed before input.

For a given coordinate system, the program sequentially fits all desired planes and lines. It stores the appropriate unit vectors for the planes and lines by plane and line number. The program can then calculate dihedral angles between all pairs of planes, lines, or plane-line combinations that are specified.

8.5 Output

The output is largely self explanatory. Specifically, the following information is given:

a. equations of the planes and lines.

b. for planes, the coordinates of the centroid.

c. perpendicular distances of each point from the least-squares planes and lines.

d. average deviations, standard deviations, etc.

e. cosines of angles between plane-plane and line-line pairs.

f. sines of angles between line-plane pairs.

Each point is numbered in the output according to loading order. Thus, the Hollerith section of the plane or line specification card (see section 8.2.c) may be used, in part, to relate the points to atom numbers or other external designations.

8.6 Limitations

a. No more than 50 points may be fitted to any plane or line.

b. No less than three points may be fitted to a plane.

c. No less than two points may be fitted to a line.

d. There may be no more than 50 planes and no more than 50 lines.

e. The number of a line or plane may not be larger than 50.

8.7 Special Subroutines Called

a. subroutine RECIP.

b. subroutine MTXMUL.

c. function DOTPRD.

8.8 Special Tape Requirements

None.

9. POINT TO PEAK DISTANCE CALCULATION

9.1 Purpose

This program provides a means for calculating distances from one or several points to a set of points in any three-dimensional coordinate system.

9.2 Input

a. 72 columns of Hollerith characters (format 12A6). These characters are used to title the output.

b. Unit Cell Card:

columns	1-10	11-20	21-30	31-40	41-50	51-60
data	a	b	c	α	β	γ
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

The quantities $a, b, c, \alpha, \beta, \gamma$ are the real-space unit cell parameters in units of angstroms and degrees.

c. Maximum distance card.

This card contains the single quantity BMX. All distances d are tabulated for which $d \leq$ BMX (format E10.4).

d. Point Card:

columns	1-10	11-20	21-30
data	XC	YC	ZC
formats	E10.4	E10.4	E10.4

XC, YC, and ZC are the fractional coordinates of the point for which distances to the set of points, specified by the coordinate cards and their transformations, are to be calculated.

e. Coordinate card

These cards contain the fractional coordinates X, Y, and Z of the basic set of points, which gives rise to a complete set via the transformations (see card below), whose distances to point XC, YC, ZC are desired. The card layout is the same as that already given for the point card above.

f. Transformation Cards:

columns	1-10	11-30	21-30	31-40	41-50	51-60
data	T1	T2	T3	U1	U2	U3
formats	E10.4	E10.4	E10.4	E10.4	E10.4	E10.4

The function of these quantities is explained in section 7.2.G.

9.3 Data Deck

a. Hollerith card.
b. unit cell card.
c. maximum distance card.
d. point card.
e. all coordinate cards.
f. blank card.
g. all transformation cards.
h. blank card.
i. additional point cards for as many calculations as desired.
j. blank card.

9.4 Method of Calculation

This program is an abbreviation of the Interatomic Distance and Angle Program (section 7). It does not provide for interpolation or angle calculation.

9.5 Output

The output of distances is essentially the same as that described for the Interatomic Distance and Angle Program (section 7.5).

9.6 Limitations

a. The complete set of points must not exceed 500 in number.

b. A maximum of 5000 distances can be accommodated.

9.7 Special Subroutines Called

a. DOTPRD.

9.8 Special Tape Requirements

None.

10. FORM FACTORS FOR THE BUSING LEAST-SQUARES REFINEMENT PROGRAM

10.1 Purpose

Provide an automatic process for preparing form factor cards used for input to the Busing least-squares refinement program ORXLS (1).

10.2 Input

a. One blank card.

b. Form Factor Parameter Card:

columns	1-8	9-16	17-24	25-32	33-40	41-46
data	A	a	B	b	C	Hollerith
formats	F8.5	F8.5	F8.5	F8.5	F8.5	A6

The quantities A, a, B, b, C are the parameters, as defined by Forsyth and Wells (3), used in calculating the form factors. The six columns of Hollerith characters are used as identification on the output cards.

10.3 Data Deck

The composition of the data deck is as follows:

a. blank card.

b. as many form factor cards as desired.

c. blank card.

10.4 Method of Calculation

The analytical approximation of Vand, Eiland, and Pepinsky (7), is used as extended by the work of Forsyth and Wells (3).

The approximations are good only as far as $(\sin\theta)/\lambda \approx 1.40$ (the range of $Mo K\alpha$ radiation).

These approximations are not recommended for highly accurate work.

10.5 Output

The form factor card images are written on logical tape 10 for peripheral punching. For each atomic species, five cards are punched as follows:

a. a blank separator card.

b. four cards containing the form factor values in intervals of 0.05 in $(\sin\theta)/\lambda$ from 1.55 to 0, in that order.

Each card has an F in column 72. Columns 73-78 contain the Hollerith characters specified in the form factor parameter cards. Column 80 contains the sequence number of the card, i.e., 1,2,3, or 4.

Essentially the same information also is printed.

10.6 Special Subroutines Called

None.

10.7 Special Tape Requirements

a. Logical tape 10 for peripheral punching.

11. VARIANCE-COVARIANCE MATRIX AND ATOMIC COORDINATE INPUT FOR THE BUSING FUNCTION AND ERROR PROGRAM

11.1 Purpose

This program produces two BCD card decks containing, respectively:

a. The variance-covariance matrix for a set of atomic position coordinates, with all covariance elements given a value of zero.

b. Atomic coordinates.

These cards are ready for input to the Busing Function and Error Program ORXFE (2).

11.2 Input

a. Preliminary Card:

columns	1-9	10-19
data	N	SF
formats	I9	E10.5

N is the order of the variance-covariance matrix, i.e., N = 3× (number of atoms).

SF is a scale factor by which the matrix is to be multiplied. Specifically, $SF = \Sigma\ w(F_0 - F_c)^2/(m - n)$, or unity.

b. Unit Cell Card:

columns	1-10	11-20	21-30
data	a	b	c
formats	E10.5	E10.5	E10.5

If the standard deviations on the cards described below are in fractional (dimensionless) form, a,b, and c all have values of one.

If the standard deviations are in units of angstroms, then a,b, and c are the unit cell edge lengths in units of angstroms.

c. Standard Deviation Card:

columns	1-10	11-20	21-30
data	σ (X)	σ (Y)	σ (Z)
formats	E10.5	E10.5	E10.5

The quantities σ(X), σ(Y), and σ(Z) are standard deviations or uncertainties of the atomic coordinates X, Y, and Z. These quantities may be dimensionless or may have units of angstroms (see section 11.2.b).

d. Coordinate card.

The layout of the coordinate cards is the same as for the standard deviation cards. Each coordinate card contains the fractional coordinates X, Y, and Z of an atom whose standard deviations are given in the corresponding card of the standard deviation deck.

11.3 Data Deck

a. preliminary card.

b. unit cell card.

c. all standard deviation cards.

d. all coordinate cards.

11.4 Output

Output may be on logical tape 9 for peripheral punching or, if sense switch 1 is down, the cards are punched on-line.

Each matrix card is numbered sequentially and identified with the letters SD (format 8E9.4, I4, 3H SD).

Each atomic coordinate card is numbered sequentially and identified with the letter P (format 8F9.6, I4, 24 P).

The two decks are separated by a blank card.

11.5 Limitations

The program will accommodate no more than 64 atoms.

11.6 Special Subroutines Called

None.

11.7 Special Tape Requirements

Logical tape 9 is used for peripheral punching.

12. OTHER FUNCTIONS AND SUBROUTINES

12.1 Function ARCSIN(X)

This program uses Hasting's Chebyshev approximation (sheet 39 of Ref. 9).

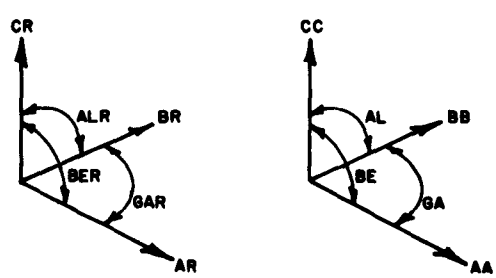
If $|X| > 1$, the program calls a subroutine ENDJOB which may be constructed by the user to suit his purposes.

The program was coded by B. A. Schoomer.*

12.2 Subroutine RECIP (AR, BR, CR, ALR, BER, GAR, AA, BB, CC, COSAL, COSBE, COSGA)

Given the sets of three translational and three angular parameters for a three-dimensional space lattice, this subroutine finds the parameters for the corresponding reciprocal space lattice.

Given Lattice: Reciprocal Lattice:



AR, BR, CR, ALR, BER, GAR ⟶ AA, BB, CC, AL, BE, GA

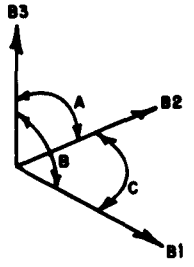
AR, BR, and CR may be given in any convenient units; ALR, BER, and GAR, are given in degrees.

*Diffraction Branch, Optics Division, NRL.

12.3 Function DOTPRD (U, V, W, X, Y, Z, B1, B2, B3, COSA, COSB, COSC)

This function calculates the scalar product of two vectors $\overline{U}$ and $\overline{V}$ where $\overline{U} = \overline{U}(U,V,W)$ and $\overline{V} = \overline{V}(X,Y,Z)$.

The vectors $\overline{U}$ and $\overline{V}$ are defined on a skew-vector basis B1, B2, B3



such that

$$\overline{U} = UB1 + VB2 + WB3$$

$$\overline{V} = XB1 + YB2 + ZB3$$

and

$$\overline{U} \cdot \overline{V} = UX(B1)^2 + VY(B2)^2 + WZ(B3)^2 + (VZ + YW)\,B2\,B3(\cos A) +$$

$$(UZ + WX)\,B1\,B3(\cos B) + (UY + VX)\,B1\,B2(\cos C).$$

12.4 Function SCAFAC (A, A1, B, B1, C, S)

This function calculates an atomic scattering factor using the analytic approximation of Vand, Eiland, and Pepinsky,(6).

The scattering factor $f(s)$ is

$$f(s) = A \exp(-A1\,S^2) + B \exp(-B1\,S^2) + C.$$

The quantities A, A1, B, B1, and C are taken from the tables of Forsyth and Wells (2). S is $(\sin \theta)/\lambda$.

12.5 Subroutine MTXMUL (L, M, N, A, B, C)

This subroutine performs matrix multiplication according to the equation

$$AB = C$$

where

the number of rows in A is L

the number of columns in A is M

the number of columns in B is N.

(As listed in this report, the dimensions of all matrices are 3 × 3; however, these may be changed to any other values needed.)

12.6 Function INTG(A)

This program converts floating point integers to fixed point integers without truncation error. This is done in a manner such that the integer value zero is not printed with a leading minus sign.

REFERENCES

1. Busing, W.R., and Levy, H.A., "A Crystallographic Least Squares Refinement Program for the IBM 704," Oak Ridge National Laboratory Central File No. 59-4-37 (1959)

2. Busing, W.R., and Levy, H.S., "A Crystallographic Function and Error Program for the IBM 704," Oak Ridge National Laboratory Central File No. 59-12-3 (1959)

3. Forsyth, J.B., and Wells, M., Acta Cryst. 12:412 (1959)

4. Hauptman, H., and Karle, J., Acta Cryst. 12:846 (1959)

5. Hauptman, H., and Karle, J., Acta Cryst. 10:267 (1957)

6. Karle, J., and Hauptman, H., Acta Cryst. 10:515 (1957)

7. Vand, V., Eiland, P.F., and Pepinsky, R., Acta Cryst. 10:303 (1957)

8. Schomaker, V., Waser, J., Marsh, R.E., and Bergman, G., Acta Cryst. 12:600 (1959)

9. Hastings, C., "Approximations for Digital Computers," Princeton:Princeton University Press (1955)

APPENDIX A

FORTRAN LISTINGS OF GENERAL UTILITY PROGRAMS APPLICABLE TO CRYSTAL STRUCTURE ANALYSIS

In the form presented in this appendix, the FORTRAN-language programs are written for use with the IBM 7090 IB Monitor system.

Least-Squares Cell Parameter

```
      DIMENSION  NAME(10),M(3,150),W(150),S(150),S2(150),SC(150),        02691
     1 H(3,3,150),G(3,3),SG(3,3),BE(3,3),AL(3,3),B(3),A(3),SA(3),SAL(3,302691
     2 ),EB(3)                                                          02691
      ITP=5
      JTP=6
   50 MM=1
      READ INPUT TAPE ITP,1000,N1,LIST,YAM,(NAME(I),I=1,10)
      IF(N1)500,500,100
  100 READ INPUT TAPE ITP,2000,M(1,MM),M(2,MM),M(3,MM),S(MM),W(MM)
      IF(XABSF(M(1,MM))+XABSF(M(2,MM))+ XABSF(M(3,MM)))140,140,110       02691
  110 S2(MM) = 4.0*(S(MM) **2)                                           02691
      IF(W(MM))120,120,130                                               02691
  120 W(MM) = S(MM)                                                      02691
  130 MM = MM +1                                                         02691
      GO TO 100                                                          02691
  140 MM=MM-1                                                            02691
      IF(YAM)145,145,141                                                 02691
  141 YAM = YAM**2                                                       02691
      DO 142 I =1,MM                                                     02691
  142 S2(I)= S2(I)/YAM                                                   02691
  145 NN = 1                                                             02691
      DO 147 I=1,3                                                       02691
      DO 147 J=1,3                                                       02691
      DO 147 K=1,MM                                                      02691
  147 H(I,J,K)=0.0                                                       02691
      GO TO(310,290,240,210,180,150),N1                                  02691
  150 N = 1                                                              02691
      DO 160 I =1,MM                                                     02691
  160 H(1,1,I)= M(1,I)**2+ M(2,I)**2+M(3,I)**2                           02691
      GO TO 325                                                          02691
  180 N=2                                                                02691
      NN=2                                                               02691
      DO 190 I =1,MM                                                     02691
      H(2,2,I)= M(3,I)**2
  190 H(1,1,I)=M(2,I)**2 + M(1,I)**2 + M(2,I)* M(1,I)
      GO TO 325                                                          02691
  210 N=2                                                                02691
      DO 220 I=1,MM                                                      02691
      H(2,2,I)= M(3,I)**2
  220 H(1,1,I)= M(2,I)**2 + M(1,I)**2
      GO TO 325                                                          02691
  240 N = 3                                                              02691
      GO TO 315                                                          02691
  290 N = 4                                                              02691
      GO TO 315                                                          02691
  310 N = 6                                                              02691
```

```
315 DO  320 I = 1,3                                                    02691
    DO  320 J = I,3                                                    02691
    DO  320 K = 1,MM                                                   02691
320 H(I,J,K) = M(I,K)* M(J,K)                                          02691
325 DO  326  I = 1,3                                                   02691
    DO  326  J = 1,3                                                   02691
    G(I,J) = 0.0                                                       02691
    SG(I,J) = 0.0                                                      02691
    BE(I,J) = 0.0                                                      02691
326 AL(I,J) = 0.0                                                      02691
    IF(MM-N)327,327,328                                                02691
327 WRITE OUTPUT TAPE JTP,3000
    GO TO 500                                                          02691
328 CALL PARAM(N,H,W,G,SG,F,SC,MM,S2,LL)                               02691
    DO  345  I =1,LL                                                   02691
    DO  345  J =1,LL                                                   02691
    IF(I -J)340,330,340                                                02691
330 B(I) = SQRTF(G(I,I))                                               02691
    GO TO 345                                                          02691
340 BE(I,J)= G(I,J)/SQRTF(G(I,I)*G(J,J))                               02691
345 CONTINUE                                                           02691
    IF(N-2)346,347,362
346 B(2)=B(1)
    G(2,2)=G(1,1)
    SG(2,2)=SG(1,1)                                                    02691
    GO TO 360                                                          02691
347 GO TO(360,350),NN                                                  02691
350 BE(1,3)= 0.5
    BE(3,1)=BE(1,3)
    G(1,3) =  0.5*G(1,1)
    G(3,1) =  G(1,3)
360 B(3)=B(1)
    G(3,3)=G(1,1)
    SG(3,3)=SG(1,1)                                                    02691
362 EB(1)=90.0 -57.29578*ARCSIN(BE(2,3))
365 EB(2)=90.0 -57.29578*ARCSIN(BE(1,3))
368 EB(3)=90.0 -57.29578*ARCSIN(BE(1,2))
369 CALL RECIP(B(1),B(2),B(3),EB(1),EB(2),EB(3),A(1),A(2),A(3),        02691
   1 AL(2,3),AL(1,3),AL(1,2))                                          02691
    CALL ERRREL(G,SG,BE,A,AL,N,SA,SAL,V,SVR,LL)                        02691
    VR = 1.0/V                                                         02691
    CALL OUTPRM(A,AL,NAME,B,EB,VR,SA,SAL,SVR,LIST,MM,N,LL,F,SC,S2,W,M
   1,N1,JTP)
    GO TO 50
500 CALL EXIT
1000 FORMAT(2I2,E8.5,10A6)                                             02691
2000 FORMAT(3I4,2E10.5)                                                02691
3000 FORMAT(1H1,3X,98H THERE ARE NOT ENOUGH  DEGREES OF FREEDOM.   UNIT02691
   1 CELL PARAMETERS AND ERRORS CANNOT BE CALCULATED.)                 02691
    END                                                                02691
```

Subroutine DET

```
C    SHARE DISTRIBUTION NO. 635
     SUBROUTINE DET(A,ALPHA,N,BET)
     DIMENSION A(6,6)
     BET=1.
     IF(N-1)400,200,300                                                02691
200  BET = A(1,1)
     GO TO 400                                                         02691
300  A(1,1)= A(1,1)- ALPHA                                             02691
6    DO 15 I=2,N                                                  DET 0005
     A(I,I)=A(I,I)-ALPHA                                          DET 0006
70   II=I-1                                                       DET 0007
```

```
7     DO 15 J=1,II                                                    DET 0008
8     IF (A(I,J))9,15,9                                               DET 0009
9     IF(ABSF(A(J,J))-ABSF(A(I,I)))11,10,10                           DET 0010
10    R=A(I,J)/A(J,J)                                                 DET 0011
      GO TO 130                                                       DET 0012
11    R=A(J,J)/A(I,J)                                                 DET 0013
      DO 12 K=1,N                                                     DET 0014
      B=A(J,K)                                                        DET 0015
      A(J,K)=A(I,K)                                                   DET 0016
12    A(I,K)=B                                                        DET 0017
      BET=-BET
130   JJ=J+1                                                          DET 0019
13    DO 14L=JJ,N                                                     DET 0020
14    A(I,L)=A(I,L)-R*A(J,L)                                          DET 0021
15    CONTINUE                                                        DET 0022
16    DO 20 I=1,N                                                     DET 0023
20    BET=BET*A(I,I)
 400  RETURN                                                            02691
      END
```

Subroutine PARAM

```
      SUBROUTINE PARAM(N,H,W,G,SG,F,SC,MM,S2,LL)                        02691
      DIMENSION H(3,3,150),W(150),G(3,3),SG(3,3),SC(150),S2(150),D(3,3),02691
     1 A(6,6),B(6),AA(6,7),X(6,1)                                       02691
      IF(N -3)362,365,365                                               02691
  362 LL = N                                                            02691
      GO TO 330                                                         02691
  365 LL = 3                                                            02691
  330 DO  360  I = 1,LL                                                 02691
      DO  360  J = 1,LL                                                 02691
      IF(I-J)350,340,350                                                02691
  340 D(I,I) = 1.0                                                      02691
      GO TO 360                                                         02691
  350 D(I,J) = 0.0                                                      02691
  360 CONTINUE                                                          02691
  367 DO 440  I =1,LL                                                   02691
      DO 440  J =I,LL                                                   02691
      DO 440  K =1,LL
      DO 440  L =K,LL                                                   02691
      IF(I - J)380,370,380                                              02691
  370 JJ = I                                                            02691
      GO TO 390                                                         02691
  380 JJ =1+I+J
  390 IF(K - L)410,400,410                                              02691
  400 KK = K                                                            02691
      GO TO 420                                                         02691
  410 KK =1+K+L
  420 A(JJ,KK)=0.0                                                      02691
      B(JJ) = 0.0                                                       02691
      DO 430 II=1,MM                                                    02691
      A(JJ,KK) = A(JJ,KK) + W(II)* H(I,J,II)*H(K,L,II)                  02691
  430 B(JJ) = B(JJ) + W(II)* S2(II)* H(I,J,II)                          02691
      A(JJ,KK) =(2.-D(I,J))    *(2.0 - D(K,L))*A(JJ,KK)
      B(JJ) = B(JJ)*(2.0 - D(I,J))                                      02691
      AA(JJ,KK)= A(JJ,KK)                                               02691
  440 AA(JJ,N+1) = B(JJ)                                                02691
      IF(N-1)445,445,446
  445 G(1,1)=B(1)  /A(1,1)
      GO TO 480
  446 CALL MATS(AA,X,N,1)                                               02691
      DO  470  I = 1,LL                                                 02691
      DO  470  J = 1,LL                                                 02691
      IF(I - J) 460,450,460                                             02691
```

```
450 G(I,I)= X(I,1)                                                    02691
    GO TO 470                                                         02691
460 K =1+I+J
    G(I,J) =  X(K,1)                                                  02691
470 CONTINUE                                                          02691
480 CALL ERRPRM(W,H,F,SC,SG,N,MM,G,S2,A,LL,D)                         02691
    RETURN                                                            02691
    END                                                               02691
```

Subroutine ERRPRM

```
    SUBROUTINE ERRPRM(W,H,F,SC,SG,N,MM,G,S2,A,LL,D)                   02691
    DIMENSION H(3,3,150),SC(150),SG(3,3),G(3,3),S2(150),A(6,6),AA(6,6 02691
   1 ),W(150),SK(6),D(3,3)                                            02691
    F = 0.0                                                           02691
    DO 490  L = 1,MM                                                  02691
    SC(L) = 0.0                                                       02691
    DO 480  I = 1,LL                                                  02691
    DO 480  J = I,LL                                                  02691
480 SC(L)=SC(L)+H(I,J,L)*G(I,J)*(2.0-D(I,J))                          02691
490 F = F + W(L)*(SC(L) - S2(L))**2                                   02691
    V = MM - N                                                        02691
    IF(N, -1)500,500,505                                              02691
500 SG(1,1)=  F/V                                                     02691
    GO TO 680                                                         02691
505 DO 506 I=1,N
    DO 506 J=1,N
506 AA(I,J) = A(I,J)
    CALL DET(AA,0.0,N,TED)
    N2 = N -1                                                         02691
    DO  640   K=1,N                                                   02691
    DO  570   I=1,N                                                   02691
    DO  570   J=1,N                                                   02691
    IF(K-I)520,570,510                                                02691
510 II = I                                                            02691
    GO TO 530                                                         02691
520 II= I - 1                                                         02691
530 IF(K - J)550,570,540                                              02691
540 JJ = J                                                            02691
    GO TO 560                                                         02691
550 JJ = J -1                                                         02691
560 AA(II,JJ) = A(I,J)                                                02691
570 CONTINUE                                                          02691
    CALL DET(AA,0.0,N2,EDT)                                           02691
640 SK(K) = (F*EDT)/(TED*V)                                           02691
    DO  670  I = 1,LL                                                 02691
    DO  670  J = 1,LL                                                 02691
    IF(I - J)660,650,660                                              02691
650 SG(I,I) = SK(I)                                                   02691
    GO TO 670                                                         02691
660 K =1+I+J
    SG(I,J) = SK(K)                                                   02691
670 CONTINUE                                                          02691
680 RETURN                                                            02691
    END                                                               02691
```

Subroutine ERRREL

```
      SUBROUTINE ERRREL(G,SG,BE,A,AL,N,SA,SAL,V,SVR,LL)                 02691
      DIMENSION G(3,3),SG(3,3),BE(3,3),A(3),AL(3,3),SA(3),SAL(3,3),U(3) 02691
      V = G(1,1)* G(2,2)* G(3,3) + 2.0* G(2,3)* G(1,3)* G(1,2)-G(1,1)*  02691
     1(G(2,3) **2)- G(2,2)*(G(1,3) **2)- G(3,3)*(G(1,2) **2)            02691
      V=SQRTF(V)
      SZ = 0.0                                                          02691
      DO 5 I=1,LL
    5 U(I)=0.0
      IF(N-1)10,10,20                                                   02691
   10 SA(1)=(SG(1,1)*(A(1)/G(1,1))**2)/2.0                              02691
      GO TO 380                                                         02691
   20 DO 310 I=1,LL                                                     02691
      DO  310   J =1,LL                                                 02691
      DO  310   K =1,LL                                                 02691
      IF(I -J)100,310,100                                               02691
  100 IF(I -K)200,310,200                                               02691
  200 IF(J-K) 300,310,310                                               02691
  300 U(I) =  2.0* SG(J,K)-((G(J,K)/(G(J,J)* G(K,K)))**2)*(SG(K,K)*(G(J,02691
     1 J) **2)+ SG(J,J)*(G(K,K) **2))                                   02691
      SZ = SZ +(G(I,I)* U(I))*(G(I,I)*(G(J,K) **2)+ G(I,J)*G(I,K)* SQRTF02691
     1 (G(J,J)*G(K,K)))                                                 02691
  310 CONTINUE                                                          02691
      SZ = SZ/(2.0 *(V**4))                                             02691
      D = 1.0                                                           02691
      IF(N-4)330,320,330                                                02691
  320 D = -D                                                            02691
  330 DO  370  I = 1,LL                                                 02691
      DO  370  J = 1,LL                                                 02691
      DO  370  K = 1,LL                                                 02691
      IF(LL-2)335,360,335
  335 IF(I-J)340,370,340                                                02691
  340 IF(I-K)350,370,350                                                02691
  350 IF(J-K)360,370,370                                                02691
  360 SA(I) =(( D*(G(J,K)/(A(I)*(V**2)))**2)* U(I) + (A(I)**2)*( SG(I,I)02691
     1/(G(I,I) **2)+  2.0*SZ))/2.0
      SAL(J,K)= (1.0 - AL(J,K)**2 )*(G(I,I)* U(I) + (BE(I,J)**2 +((BE(I,02691
     1 K)**2)*(1.0- BE(I,J)**2)*(AL(J,K)**2))/(1.0 - BE(I,K)**2)) * G(J,02691
     2 J)* U(J)  +  (BE(I,K)**2 +((BE(I,J)**2)*(1.0 - BE(I,K)**2)*(AL(J,02691
     3 K)**2))/(1.0 - BE(I,J)**2))* G(K,K)* U(K))/(2.0*(V**2))          02691
  370 CONTINUE                                                          02691
  380 SVR=SZ*2.0                                                        02691
  420 DO  430  I = 1,3                                                  02691
  430 SVR = SVR + SG(I,I)/( G(I,I)**2)                                  02691
      DO  435  I =1,LL                                                  02691
  435 SA(I) = SQRTF(SA(I))                                              02691
  440 SVR= SQRTF(SVR/((V**2)*2.))
      RETURN                                                            02691
      END                                                               02691
```

Subroutine OUTPRM

```
      SUBROUTINE OUTPRM(A,AL,NAME,B,EB,VR,SA,SAL,SVR,LIST,MM,N,LL,F,SC, 02691
     1S2,W,M,N1,JTP)
      DIMENSION NAME(10),M(3,150),W(150),S2(150),SC(150),AL(3,3),B(3),  02691
     1A(3),SA(3),SAL(3,3),EB(3),ALD(3),SALD(3)                          02691
      IF(N-4)95 ,50,50
   50 DO  100  I =1,2
      K = I +1                                                          02691
      DO  100  J =K,3                                                   02691
      L = 6-I-J                                                         02691
   60 ALD(L)= 90.0 - 57.295780* ARCSIN(AL(I,J))
```

```
 70 D = SQRTF(SAL(I,J))                                                    02691
100 SALD(L)= 57.295780*ABSF(ABSF(ARCSIN(AL(I,J)+D))-ABSF(ARCSIN(AL(I,J02691
   1)-D)))
 95 WRITE OUTPUT TAPE JTP,1000,(NAME(I),I=1,10),MM                         02691
    DO 170 I= 1,N
    GO TO(101,102, 96),LL
 96 IF(N-4)103,97,103
 97 GO TO(110,120,130,160),I
101 GO TO 110                                                              02691
102 GO TO(110,125),I                                                       02691
103 GO TO(110,120,130,140,150,160),I
130 WRITE OUTPUT TAPE JTP,1100,B(3),A(3),SA(3)
    GO TO 170                                                              02691
120 WRITE OUTPUT TAPE JTP,1200,B(2),A(2),SA(2)
    GO TO 170                                                              02691
125 WRITE OUTPUT TAPE JTP,1100,B(2),A(2),SA(2)
    GO TO 170                                                              02691
110 WRITE OUTPUT TAPE JTP,1300,B(1),A(1),SA(1)
    GO TO 170                                                              02691
160 WRITE OUTPUT TAPE JTP,1400,EB(3),ALD(3),SALD(3)
    GO TO 170                                                              02691
150 WRITE OUTPUT TAPE JTP,1500,EB(2),ALD(2),SALD(2)
    GO TO 170                                                              02691
140 WRITE OUTPUT TAPE JTP,1600,EB(1),ALD(1),SALD(1)
170 CONTINUE                                                               02691
    WRITE OUTPUT TAPE JTP,1700,VR,SVR
    WRITE OUTPUT TAPE JTP,1800
    GO TO(500,510,520,530,540,550),N1                                      02691
500 WRITE OUTPUT TAPE JTP,2400
    GO TO 175                                                              02691
510 WRITE OUTPUT TAPE JTP,2500
    GO TO 175                                                              02691
520 WRITE OUTPUT TAPE JTP,2600
    GO TO 175                                                              02691
530 WRITE OUTPUT TAPE JTP,2700
    GO TO 175                                                              02691
540 WRITE OUTPUT TAPE JTP,2800
    GO TO 175                                                              02691
550 WRITE OUTPUT TAPE JTP,2900
175 IF(LIST)260,180,260                                                    02691
180 R = MM - N                                                             02691
    SD = SQRTF(F/R)                                                        02691
    SD2 = SD* 2.5                                                          02691
    L1 = MM/20                                                             02691
    L2 = MM - L1*20                                                        02691
    L3 = 0                                                                 02691
185 L3 =L3+1                                                               02691
    IF(L1 - L3)200,190,190                                                 02691
190 K2 = L3*20                                                             02691
    K1 = K2 -19                                                            02691
    GO TO 220                                                              02691
195 L3=L3+1                                                                02691
200 IF(L2)260,260,210                                                      02691
210 K1 = L1*20 +1                                                          02691
    K2 = K1 + L2 -1                                                        02691
220 NM = 0                                                                 02691
    WRITE OUTPUT TAPE JTP,2000,L3,SD
    DO 250  I = K1,K2                                                      02691
    DEL =(S2(I)-SC(I))*SQRTF(W(I))                                         02691
    IF(SD2-ABSF(DEL))230,230,240                                           02691
230 NM = 1                                                                 02691
    WRITE OUTPUT TAPE JTP,2100,M(1,I),M(2,I),M(3,I),S2(I),SC(I),W(I),
   1DEL
    GO TO 250                                                              02691
```

```
 240 WRITE OUTPUT TAPE JTP,2200,M(1,I),M(2,I),M(3,I),S2(I),SC(I),W(I),
    1DEL
 250 CONTINUE                                                          02691
     IF(NM)256,256,255                                                 02691
 255 WRITE OUTPUT TAPE JTP,2300
 256 IF(L1-L3)260,195,185                                              02691
 260 RETURN                                                            02691
1000 FORMAT(1H1/1H4,36X,45HUNIT CELL PARAMETERS WITH STANDARD DEVIATION02691
    1S//29X,10A6//46X,23HNUMBER OF REFLECTIONS =,I6//)                 02691
1100 FORMAT(1HO,26X,5H C* =,F10.7,22X,4H C =,F9.5,6H  +OR-,F8.5/)      02691
1200 FORMAT(1HO,26X,5H B* =,F10.7,22X,4H B =,F9.5,6H  +OR-,F8.5/)      02691
1300 FORMAT(1HO,26X,5H A* =,F10.7,22X,4H A =,F9.5,6H  +OR-,F8.5/)      02691
1400 FORMAT(1HO,23X,8HGAMMA* =,F10.5,19X,7HGAMMA =,F9.4,6H  +OR-,F8.4/)02691
1500 FORMAT(1HO,23X,8H BETA* =,F10.5,19X,7H BETA =,F9.4,6H  +OR-,F8.4/)02691
1600 FORMAT(1HO,23X,8HALPHA* =,F10.5,19X,7HALPHA =,F9.4,6H  +OR-,F8.4/)02691
1700 FORMAT(1HO,64X,3HV =,F11.4,6H  +OR-,F10.4////)                   02691
1800 FORMAT(33X,48HUNITS ARE  1/(ANGSTROMS), ANGSTROMS, AND DEGREES)   02691
2100 FORMAT(1HO,11X,3I6,6X,E14.7,5X,E14.7,3X,E12.5,6X,E12.5,3H  *)     02691
2200 FORMAT(1HO,11X,3I6,6X,E14.7,5X,E14.7,3X,E12.5,6X,E12.5)           02691
2000 FORMAT(1H1,45X,25HOBSERVED AND CALCULATED S,25X,5HPAGE ,I3///27X,102691
    18HS = (2*SIN()/L)**2,10X,21HSTANDARD DEVIATION = ,E12.5///17X,13HH02691
    2     K     L,10X,6HS(OBS),13X,6HS(CAL),12X,1HW, 9X,18H(DELTA S)*(W02691
    3**1/2))                                                           02691
2300 FORMAT(1HO/9X,58H*  THIS DEVIATION IS GREATER THAN 2.5*(STANDARD D02691
    1EVIATION))                                                        02691
2400 FORMAT(1HO,45X,27HTHE CRYSTAL IS TRICLINIC   )                    02691
2500 FORMAT(1HO,45X,27HTHE CRYSTAL IS MONOCLINIC  )                    02691
2600 FORMAT(1HO,45X,27HTHE CRYSTAL IS ORTHORHOMBIC)                    02691
2700 FORMAT(1HO,45X,27HTHE CRYSTAL IS TETRAGONAL  )                    02691
2800 FORMAT(1HO,45X,27HTHE CRYSTAL IS HEXAGONAL   )                    02691
2900 FORMAT(1HO,45X,27HTHE CRYSTAL IS CUBIC       )                    02691
     END                                                               02691
```

Quasi Normalization of Structure Factors

```
CSFQNOR   QUASI NORM. OF STRUCT. FACTORS USING F TAPE INPUT
     DIMENSION NME(12),  AS(20),AS1(20),BS(20),BS1(20),CS(20),AN(20),  02691
    1 H1(500),H2(500),H3(500),M1(500),M2(500),M3(500),AVEQ(500),SI(500)02691
     ITP=5
     JTAPE =  15                                                       02691
     ITAPE =  16                                                       02691
     REWIND ITAPE                                                      02691
     REWIND JTAPE                                                      02691
     READ INPUT TAPE ITP,
    1     1000,NOIB,NASP,NF,BT1,EX     ,LIB
     READ INPUT TAPE ITP,
    1     40,(AS(I),AS1(I),BS(I),BS1(I),CS(I),AN(I),I=1,NASP)
     IF(NF)5,5,1
   1 DO 2 I=1,NF
   2 CALL FLSKPD(ITAPE)
   5 IF(LIB)10,30,10
  10 READ INPUT TAPE ITAPE,1200,(NME(I),I=1,12)
  30 NO = 0                                                            02691
     N1 = NOIB/500                                                     02691
     WRITE OUTPUT TAPE JTAPE,740,NOIB                                  02691
 100 IF(N1-NO)400,150,200                                              02691
 150 N4 = NOIB - N1* 500                                               02691
     IF(N4)400,400,210                                                 02691
 200 N4 = 500                                                          02691
```

```
 210 READ INPUT TAPE ITAPE,1100,(H1(I),H2(I),H3(I),AVEQ(I),SI(I),I= 1, 02691
    1 N4)                                                              02691
     DO  300  I =  1,N4                                                02691
     M1(I)= INTG(H1(I))                                                02691
     M2(I)= INTG(H2(I))                                                02691
     M3(I)= INTG(H3(I))                                                02691
     SI(I)= SI(I)**2                                                   02691
     SIG = 0.0                                                         02691
     DO  250  J = 1,NASP                                               02691
 250 SIG=SIG+AN(J)*(AS(J)*EXPF(-AS1(J)*SI(I))+ BS(J)*EXPF(-BS1(J)*SI(I)02691
    1)+CS(J))**2                                                       02691
 300 AVEQ(I)=(AVEQ(I)* EXPF(BT1*(SI(I)**EX))/SIG)- 1.0                 02691
     WRITE OUTPUT TAPE JTAPE,680,(M1(I),M2(I),M3(I),AVEQ(I),I =1,N4)   02691
     NO = NO +1                                                        02691
     GO TO 100                                                         02691
 400 REWIND ITAPE                                                      02691
     END FILE JTAPE                                                    02691
     REWIND JTAPE                                                      02691
     PRINT 2000                                                        02691
     CALL   EXIT
1000 FORMAT(3I10,2E10.4,I10)
  40 FORMAT(5F8.4,F4.0)                                                02691
1100 FORMAT(4F9.2,18X,F9.6)                                            02691
 680 FORMAT(3I4,F20.5)                                                 02691
2000 FORMAT( 16H     JOB FINSHED.////////////)
 740 FORMAT(I7)                                                        02691
1200 FORMAT(12A6)
     END
```

Rational Dependence

```
CRATDEP     RATIONAL DEPENDANCE (AFTER BLOCK-YANNONI)
     DIMENSION NAME(12), NF(29),KA(28),KB(28),
    1KC(28),EC(29),MK(5000),ML(5000),MH(5000),ESQM(5000),MR(5000)
     COMMON MH,MK,ML,ESQM,MR,KA,KB,KC,JNF,MAD,M,IT,NAME,N,J,K,MA,JTP,
    1AVESQG,JPUT,NCTR,NO
     KA(1) = 0                                                          06800
     KA(2) = 1                                                          06800
     KA(3) =-1                                                          06800
     KA(4) = 2                                                          06800
     KA(5) =-2                                                          06800
     KA(6) = 3                                                          06800
     KA(7) =-3                                                          06800
     KA(8) = 4                                                          06800
     KA(9) =-4                                                          06800
     KA(10) = 5                                                         06800
     KA(11) =-5                                                         06800
     KA(12) = 6                                                         06800
     KA(13) =-6                                                         06800
     KA(14) = 7                                                         06800
     KA(15) =-7                                                         06800
     KA(16) = 8                                                         06800
     KA(17) =-8                                                         06800
     KA(18) = 9                                                         06800
     KA(19) =-9                                                         06800
     KA(20) = 10                                                        06800
     KA(21) =-10                                                        06800
     KA(22) = 11                                                        06800
     KA(23) =-11                                                        06800
     KA(24) = 12                                                        06800
     KA(25) =-12                                                        06800
     KA(26) = 13                                                        06800
     KA(27) =-13                                                        06800
     KA(28) = 14                                                        06800
     ITP=5
     JTP=6
     KTP=12
     REWIND KTP
  50 READ INPUT TAPE ITP,8,(NAME(I),I=1,12)
     READ INPUT TAPE ITP,4,NA,NINT,NFIN,MINN,AN,SDMIN,JPUT
  60 READ INPUT TAPE KTP,5,NO
  61 READ INPUT TAPE KTP,6,(MH(J),MK(J),ML(J),ESQM(J),J=1,NO)
     REWIND KTP
     SUMESQ=0.0
     DO 62 I=1,NO
     ESQM(I)=ESQM(I)+1.0
  62 SUMESQ=SUMESQ+ESQM(I)
     BNO=NO
     AVESQ=SUMESQ/BNO
  70 MA=NINT
     NCTR=-1
     WRITE OUTPUT TAPE JTP,15,(NAME(J),J=1,12),NINT,NFIN,AVESQ,AN,MINN,
    1NO,SDMIN
  80 IF(NA)83,90,90                                                     06800
  83 AN=1.414214*AN                                                     06800
  90 DO 95  J= 1,28
  92 KB(J)=KA(J)                                                        06800
  95 KC(J)=KA(J)                                                        06800
 180 DO 440 N=1,MA                                                      06800
 190 DO 440 J=1,MA                                                      06800
 200 DO 440 K=1,MA                                                      06800
     N=N
     J=J
     K=K
     IF(KA(N)) 440,2000,202
```

```
2000 IF(KB(J))440,2010,202
2010 IF(KC(K))440,440,202
 202 MAD=MA+1
     DO 207 LD=1,MAD
     NF(LD)=0
 207 EC(LD)=0.
2100 DO 2400 L=1,NO
     KSUM=KA(N)*MH(L)+KB(J)*MK(L)+KC(K)*ML(L)
     MT=XMODF(KSUM,MA)
     IF(MT)2200,2300,2300
2200 MT=MT+MA
2300 MT=MT+1
     MR(L)=MT
     EC(MT)=ESQM(L)+EC(MT)
2400 NF(MT)=NF(MT)+1
 300 PMA=MA
 301 PMA=PMA/2.
 302 MAN=PMA
 303 MAN=MAN+1
 304 IT=MA+2
 310 DO 430 M=1,MAN
 311 IT=IT-1
1315 IF(IT-M) 1320,1321,1325
1320 STOP 0066
1321 DNF=NF(M)
     JNF=NF(M)
1322 BEC=EC(M)
1323 GO TO 1350
1325 JNF=NF(M)+NF(IT)
1330 DNF=JNF
1340 BEC=EC(M)+EC(IT)
1350 IF(JNF-MINN)430,430,1355
1355 AVESQG=BEC/DNF
1360 CHEK=AN/SQRTF(DNF)
     IF(CHEK-SDMIN)1365,1370,1370
1365 CHEK=SDMIN
1370 PHEK=AVESQ+CHEK
1380 PMHEK=AVESQ-CHEK
 360 IF(AVESQG-PHEK) 370,380, 380                                  06800
 370 IF(AVESQG-PMHEK)380, 380, 430
 380 IF (MA-3)400,400,3193
3193 IR = 0                                                        06800
3194 CAT=2.0                                                       06800
3200 XMA=MA                                                        06800
3210 XLA=XMA/CAT                                                   06800
3215 IZ=0                                                          06800
3220 MX=XLA                                                        06800
3230 YMX=MX                                                        06800
3240 IF (YMX-XLA) 3350,3250,3350                                   06800
3250 XKE=KA(N)                                                     06800
3260 AAD=XKE/CAT                                                   06800
3270 MAC=AAD
3280 ABD=MAC
3290 IF(ABD-AAD) 3350,3300,3350                                    06800
3300 IZ=IZ+1                                                       06800
3310 GO TO (3320,3330,3340,430),IZ
3320 XKE=KB(J)                                                     06800
3325 GO TO 3260                                                    06800
3330 XKE=KC(K)                                                     06800
3335 GO TO 3260                                                    06800
3340 XKE =M-1
3345 GO TO 3260                                                    06800
3350 IR=IR+1                                                       06800
3355 IF(MA-IR-3) 400,400,3360                                      06800
3360 CAT=CAT+1.                                                    06800
```

```
3365 IF(CAT-14.0) 3210,3210,400
 400 CALL OUTRAT
 430 CONTINUE
     IF(SENSE SWITCH 2)510,440
 440 CONTINUE                                                    06800
 450 MA=MA+1                                                     06800
 460 IF(NFIN-MA) 470,180,180
 470 READ INPUT TAPE ITP,4,NA,NINT,NFIN,MINN,AN,SDMIN,JPUT
     IF(NINT)500,500,70
 500 CALL EXIT
 510 WRITE OUTPUT TAPE JTP,9,(NAME(L2),L2=1,12)
     WRITE OUTPUT TAPE JTP,7,KA(N),KB(J),KC(K),MA
     WRITE OUTPUT TAPE JTP,16
     GO TO 500
   8 FORMAT (12A6)
   4 FORMAT (4I10,2E10.4,I10)
   5 FORMAT (I7)
   6 FORMAT(3I4,F20.5)
   7 FORMAT(6H0  A =I3,6X,3HB =I3,6X,3HC =I3,6X,6HMODE =I6)
   9 FORMAT (1H1,19X,12A6)
  15 FORMAT(1H2,19X,12A6////20X,16HINITAL MODULAS =I6,10X,15HFINAL MODU
     1LAS =I6///20X,19HAVERAGE  E**2      =F9.5///20X, 13HDEVIATIONS OFF7
     2.3, 66H STANDARD DEVIATIONS FROM AVE   E**2    ARE CONSIDERED SIGN
     3IFICANT///20X, 40HONLY SUBGROUPS CONTAINING NO FEWER THAN I6,
     4 39H REFLECTIONS ARE CONSIDERED SIGNIFICANT///20X, 10HTHERE ARE I7
     5, 30H REFLECTIONS ON THE INPUT TAPE///20X,51HTHE MINIMUM ACCEPTED
     6DEVIATION FROM AVE.  E**2  IS F5.3)
  16 FORMAT(1H0,19X,47HCALCULATION TERMINATED BY SENSE SWITCH CONTROL.)
     END
```

Subroutine OUTRAT

```
     DIMENSION NAME(12), NF(29),KA(28),KB(28),
    1KC(28),EC(29),MK(5000),ML(5000),MH(5000),ESQM(5000),MR(5000),
    2LH(40),LK(40),LL(40),ESQL(40)
     COMMON MH,MK,ML,ESQM,MR,KA,KB,KC,JNF,MAD,M,IT,NAME,N,J,K,MA,JTP,
    1AVESQG,JPUT,NCTR,NO
     KET=M-1
     IF(JPUT)75,50,75
  50 NCTR=NCTR+1
     IF(NCTR-(NCTR/9)*9)60,55,60
  55 WRITE OUTPUT TAPE JTP,9,(NAME(L2),L2=1,12)
  60 WRITE OUTPUT TAPE JTP,8,KA(N),KB(J),KC(K),MA,KET,   AVESQG,JNF
     GO TO 350
  75 NP=0
     L4=0
     DO 220 L9=1,NO
     L9=L9
     IF(MR(L9)-M)200,210,200
 200 IF(MR(L9)-IT)220,210,220
 210 L4=L4+1
     LH(L4)=MH(L9)
     LK(L4)=MK(L9)
     LL(L4)=ML(L9)
     ESQL(L4)=ESQM(L9)
     IF(40-L4)230,230,220
 220 CONTINUE
 230 J1=L4/40
     J2=L4-J1*40
     J3=J2-20
     IF (J3)241,241,243
 241 J4=J2
     GO TO 245
```

```
243 J4=J2-2*J3
    GO TO 247
245 IF (J1)300,300,246
246 J5=J1
    GO TO 250
247 J5=J1+1
250 DO 290 L1=1,J5
    NP=NP+1
    WRITE OUTPUT TAPE JTP,9,(NAME(L2),L2=1,12)
    WRITE OUTPUT TAPE JTP,7,KA(N),KB(J),KC(K),MA,KET,NP,AVESQG,JNF
    L5=L1*40-39
    IF (J1-L1)260,270,270
260 L6=L5+J3-1
    GO TO 280
270 L6=L5+19
280 DO 290 L2=L5,L6
    AQ=ESQL(L2)-1.0
    AQA=ESQL(L2)-AVESQG
    AQ1=ESQL(L2+20)-1.0
    AQA1=ESQL(L2+20)-AVESQG
    WRITE OUTPUT TAPE JTP,10
290 WRITE OUTPUT TAPE JTP,11,LH(L2),LK(L2),LL(L2),AQ,AQA,LH(L2+20),
   1LK(L2+20),LL(L2+20),AQ1,AQA1
300 IF (J4)360,360,310
310 IF (J3)320,320,315
315 L5=L6+1
    GO TO 335
320 NP=NP+1
    WRITE OUTPUT TAPE JTP,9,(NAME(L2),L2=1,12)
    WRITE OUTPUT TAPE JTP,7,KA(N),KB(J),KC(K),MA,KET,NP,AVESQG,JNF
330 L5=L6+21
335 L6=L5+J4-1
    DO 340 L2=L5,L6
    AQ=ESQL(L2)-1.0
    AQA=ESQL(L2)-AVESQG
340 WRITE OUTPUT TAPE JTP,12,LH(L2),LK(L2),LL(L2),AQ,AQA
350 RETURN
360 L4=0
    IF(NO-L9)350,350,220
  7 FORMAT(6H0  A =I3,6X,3HB =I3,6X,3HC =I3,6X,6HMODE =I6,8X,11HREMAIN
   1DER =I6,24X,4HPAGEI5///22X,10HAVE E**2 =F10.5,8X,11HNO. REFL. =I6/
   2///2(60H    H   K   L        E**2 - 1        E**2 - A
   3  ))
  8 FORMAT(6H0  A =I3,6X,3HB =I3,6X,3HC =I3,6X,6HMODE =I6,8X,11HREMAIN
   1DER =I6,24X,6H      ///22X,10HAVE E**2 =F10.5,8X,11HNO. REFL. =I6)
  9 FORMAT (1H1,19X,12A6)
 10 FORMAT (1H )
 11 FORMAT (2(1X,3I4,7X,F9.5,7X,F9.5,15X))
 12 FORMAT (1H0,3I4,7X,F9.5,7X,F9.5)
    END
```

Sigma-2 Listings

```
CSIGEXC SIGMA-2 INTERACTION EXC
    DIMENSION M1(2400),M2(2400),M3(2400),AV(2400),K1(2400),K2(2400),K3
   1(2400),QAV(2400)
    COMMON M1,M2,M3,AV
    ITP=5
    IP =11
    L=0
    READ INPUT TAPE ITP,
   1     1002,Z,IZ,NOIB
    IF(IZ) 2, 1,2                                              02691
```

```
    1 MM=2                                                          02691
      REWIND IP
      READ INPUT TAPEIP,1001,NRT
      GO TO 3                                                       02691
    2 MM=1                                                          02691
      READ INPUT TAPE ITP,1001,NRT
    3 DO 25 I=1,NRT                                                 02691
   20 GO TO(5,6),MM
    5 READ INPUT TAPE ITP,
     1     1000,N1,N2,N3,Q
      GO TO 7                                                       02691
    6 READ INPUT TAPEIP,1000,N1,N2,N3,Q
    7 CALL REJVEC(N1,N2,N3, Q)
      IF(Q-Z)25,10,10
   10 L=L+1                                                         02691
      M1(L)=N1
      M2(L)=N2
      M3(L)=N3
      AV(L)=SQRTF(1.0+Q)
   25 CONTINUE                                                      02691
   30 DO 160 J=1,L
   40 DO 70 K=1,L
   50 IF(AV(K))70,60,60
   60 BAV=AV(K)
      GO TO 80
   70 CONTINUE
   80 DO 110 I=K,L
   90 IF(AV(I)-BAV)110,100,100
  100 BAV=AV(I)
      I1=I
  110 CONTINUE
      K1(J)=M1(I1)
      K2(J)=M2(I1)
      K3(J)=M3(I1)
      QAV(J)=AV(I1)
      AV(I1)=-1.0
  160 CONTINUE
      IF(NOIB)165,180,170
  165 NOIB=L
  170 CALL SIGVEC(NOIB,K1,K2,K3,QAV,L)                              02693
  180 CALL EXIT
 1000 FORMAT(3I4,F20.5)
 1001 FORMAT(I7)
 1002 FORMAT(E10.4,2I10)
      END
```

Subroutine OUTSIG

```
      SUBROUTINE OUTSIG(M1,M2,M3,Q,N1,N2,N3,                        02693
     1Q1,QQ,N,K1,K2,K3,I,QAV)                                       02693
      DIMENSION K1(2400),K2(2400),K3(2400),                         02693
     1QAV(2400),M1(1000),M2(1000),M3(1000),Q(1000),                 02693
     2N1(1000),N2(1000),N3(1000),Q1(1000),QQ(1000)                  02693
      COMMON M1,M2,M3,Q,N1,N2,N3,Q1,QQ                              02693
      JTP=6
      IF(N)25,25,50                                                 02693
   25 K=1
      WRITE OUTPUT TAPE JTP,
     1     1000,K,K1(I),K2(I),K3(I),QAV(I)
      GO TO 130                                                     02693
   50 J=N/20                                                        02693
      IF(J)120,120,100                                              02693
```

```
 100 DO 110 I1=1,J                                                      02693
     J3=20*I1                                                           02693
     J2=J3-19                                                           02693
     WRITE OUTPUT TAPE JTP,
    1       1000,I1,K1(I),K2(I),K3(I),QAV(I)
 110 WRITE OUTPUT TAPE JTP,
    1       2000,(M1(J1),M2(J1),M3(J1),Q(J1),
    2N1(J1),N2(J1),N3(J1),Q1(J1),QQ(J1),J1=J2,J3)
     IF(N-20*J)130,130,120                                              02693
 120 I2=20*J+1                                                          02693
     I4=J+1                                                             02693
     WRITE OUTPUT TAPE JTP,
    1       1000,I4,K1(I),K2(I),K3(I),QAV(I)
     WRITE OUTPUT TAPE JTP,
    1       2000,(M1(J1),M2(J1),M3(J1),Q(J1),
    2N1(J1),N2(J1),N3(J1),Q1(J1),QQ(J1),J1=I2,N)
 130 RETURN                                                             02693
1000 FORMAT(1H1,17X,9HH   K   L,9X,1HE,13X,5HPAGE ,I2///16X,3I4,4X,F8.5
    1////70H  H(I) K(I) L(I)      E(I)    H(J) K(J) L(J)      E(J)
    2E(I)*E(J)*E)
2000 FORMAT(1H0,I4,2I5,4X,F8.5,1X,3I5,4X,F8.5,4X,F10.5)
     END                                                                02693
```

Subroutine REJVEC

```
     SUBROUTINE REJVEC(N1,N2,N3,Q)
C    DUMMY
 100 RETURN
     END

     SUBROUTINE REJVEC(N1,N2,N3,Q)
C    REJECTS ALL REFL. FOR WHICH ANY OF H,K,L EQUAL ZERO
     IF(N1)10,30,10
  10 IF(N2)20,30,20
  20 IF(N3)40,30,40
  30 Q=-10.
  40 RETURN
     END
```

Subroutine SIGVEC, Triclinic

```
C    TRICLINIC
     SUBROUTINE SIGVEC(NOIB,K1,K2,K3,QAV,L)                             02693
     DIMENSION K1(2400),K2(2400),K3(2400),                              02693
    1QAV(2400),M1(1000),M2(1000),M3(1000),Q(1000),                      02693
    2N1(1000),N2(1000),N3(1000),Q1(1000),QQ(1000)                       02693
     COMMON M1,M2,M3,Q,N1,N2,N3,Q1,QQ                                   02693
     DO 170 I=1,NOIB                                                    02693
     N=0                                                                02693
     DO 160 J=1,L                                                       02693
     DO 160 K=J,L                                                       02693
     IF(K1(J)+K1(K)-K1(I)) 10, 40, 10
  10 IF(K1(J)+K1(K)+K1(I)) 20, 50, 20
  20 IF(K1(J)-K1(K)-K1(I)) 30, 60, 30
  30 IF(K1(J)-K1(K)+K1(I))160, 70,160
  40 IF(K2(J)+K2(K)-K2(I))160, 80,160
  50 IF(K2(J)+K2(K)+K2(I))160, 90,160
  60 IF(K2(J)-K2(K)-K2(I))160,100,160
  70 IF(K2(J)-K2(K)+K2(I))160,110,160
  80 IF(K3(J)+K3(K)-K3(I))160,150,160
  90 IF(K3(J)+K3(K)+K3(I))160,150,160
 100 IF(K3(J)-K3(K)-K3(I))160,150,160
```

```
110 IF(K3(J)-K3(K)+K3(I))160,150,160
150 N=N+1
    M1(N)=K1(J)
    M2(N)=K2(J)
    M3(N)=K3(J)
    Q(N) = QAV(J)                                          02693
    N1(N)=K1(K)
    N2(N)=K2(K)
    N3(N)=K3(K)
    Q1(N)= QAV(K)                                          02693
    QQ(N)= QAV(J)* QAV(K)*QAV(I)
160 CONTINUE                                               02693
170 CALL OUTSIG(M1,M2,M3,Q,N1,N2,N3,Q1,QQ,N,
   1 K1,K2,K3,I,QAV)
    RETURN                                                 02693
    END                                                    02693
```

Subroutine SIGVEC, Monoclinic

```
C   MONOCLINIC, SECOND SETTING
    SUBROUTINE SIGVEC(NOIB,K1,K2,K3,QAV,L)                 02693
    DIMENSION K1(2400),K2(2400),K3(2400),                  02693
   1QAV(2400),M1(1000),M2(1000),M3(1000),Q(1000),          02693
   2N1(1000),N2(1000),N3(1000),Q1(1000),QQ(1000)           02693
    COMMON M1,M2,M3,Q,N1,N2,N3,Q1,QQ                       02693
    DO 170 I=1,NOIB                                        02693
    N=0                                                    02693
    DO 160 J=1,L                                           02693
    DO 160 K=J,L                                           02693
    IF(XABSF(K2(J)+K2(K))-XABSF(K2(I))) 10, 20, 10
 10 IF(XABSF(K2(J)-K2(K))-XABSF(K2(I)))160, 20,160
 20 IF(K1(J)+KI(K)-K1(I)) 30, 60,30
 30 IF(K1(J)+K1(K)+K1(I)) 40, 70,40
 40 IF(K1(J)-K1(K)-K1(I)) 50, 80,50
 50 IF(K1(J)-K1(K)+K1(I))160, 90,160
 60 M=1
    IF(K3(J)+K3(K)-K3(I))100,150,100
 70 M=2
    IF(K3(J)+K3(K)+K3(I))100,150,100
 80 IF(K3(J)-K3(K)-K3(I))146,150,146
 90 IF(K3(J)-K3(K)+K3(I))160,150,160
100 IF(K1(J))120,110,120
110 GO TO(140,145),M
120 IF(K1(K))160,130,160
130 GO TO(145,140),M
140 IF(K3(J)-K3(K)+K3(I))160,150,160
145 IF(K3(J)-K3(K)-K3(I))160,150,160
146 IF(K1(I))160,90,160
150 N=N+1
    M1(N)=K1(J)
    M2(N)=K2(J)
    M3(N)=K3(J)
    Q(N) = QAV(J)                                          02693
    N1(N)=K1(K)
    N2(N)=K2(K)
    N3(N)=K3(K)
    Q1(N)= QAV(K)                                          02693
    QQ(N)= QAV(J)* QAV(K)*QAV(I)
160 CONTINUE                                               02693
170 CALL OUTSIG(M1,M2,M3,Q,N1,N2,N3,Q1,QQ,N,
   1 K1,K2,K3,I,QAV)
    RETURN                                                 02693
    END                                                    02693
```

Subroutine SIGVEC, Orthorhombic

```
      ORTHORHOMBIC
      SUBROUTINE SIGVEC(NOIB,K1,K2,K3,QAV,L)                          02693
      DIMENSION K1(2400),K2(2400),K3(2400),                           02693
     1QAV(2400),M1(1000),M2(1000),M3(1000),Q(1000),                   02693
     2N1(1000),N2(1000),N3(1000),Q1(1000),QQ(1000)                    02693
      COMMON M1,M2,M3,Q,N1,N2,N3,Q1,QQ                                02693
      DO 170 I=1,NOIB                                                 02693
      N=0                                                             02693
      DO 160 J=1,L                                                    02693
      DO 160 K=J,L                                                    02693
      IF(XABSF(K1(J)+K1(K))-XABSF(K1(I)))100,110,100
  100 IF(XABSF(K1(J)-K1(K))-XABSF(K1(I)))160,110,160
  110 IF(XABSF(K2(J)+K2(K))-XABSF(K2(I)))120,130,120
  120 IF(XABSF(K2(J)-K2(K))-XABSF(K2(I)))160,130,160
  130 IF(XABSF(K3(J)+K3(K))-XABSF(K3(I)))140,150,140
  140 IF(XABSF(K3(J)-K3(K))-XABSF(K3(I)))160,150,160
  150 N=N+1
      M1(N)=K1(J)
      M2(N)=K2(J)
      M3(N)=K3(J)
      Q(N) = QAV(J)                                                   02693
      N1(N)=K1(K)
      N2(N)=K2(K)
      N3(N)=K3(K)
      Q1(N)= QAV(K)                                                   02693
      QQ(N)= QAV(J)* QAV(K)*QAV(I)
  160 CONTINUE                                                        02693
  170 CALL OUTSIG(M1,M2,M3,Q,N1,N2,N3,Q1,QQ,N,
     1 K1,K2,K3,I,QAV)
      RETURN                                                          02693
      END                                                             02693
```

Triple Product Summation, Centrosymmetric

```
CORTHTP  ORTHORHOMBIC TRIP. PROD. PROG. FOR CENTRO. CRYST.
      DIMENSION E(30,10,30)
      ITP=5
      JTP=6
      KTP=9
      REWIND KTP
      B=1.0E-21
      READ INPUT TAPE ITP,1000,NA,IM,JM,KM
 1000 FORMAT(6I10)
      DO 75 I=1,IM
      DO 75 J=1,JM
      DO 75 K=1,KM
   75 E(I,J,K)=B
      READ INPUT TAPE KTP,2000,NOIB
 2000 FORMAT(I7)
      DO 8 NO=1,NOIB
      READ INPUT TAPE KTP,2100,I,J,K,A
 2100 FORMAT(3I4,F20.5)
      IF(I)1,8,2
    1 I=-I
    2 IF(J)3,8,4
    3 J=-J
    4 IF(K)5,8,6
    5 K=-K
    6 E(I,J,K)=A
```

```
  8 CONTINUE
    REWIND KTP
    AN=NA
    SF=SQRTF(AN**3)/8.0
    JJJ=0
    MN=0
C   START NEW TP CALC.
  9 READ INPUT TAPE ITP,1000,M1,M2,M3,N1,N2,N3
    JJJ=JJJ+1
    I1=XABSF(M1)
    I2=XABSF(M2)
    I3=XABSF(M3)
    J1=XABSF(N1)
    J2=XABSF(N2)
    J3=XABSF(N3)
    L1=M1+N1
    L2=M2+N2
    L3=M3+N3
    K1=XABSF(L1)
    K2=XABSF(L2)
    K3=XABSF(L3)
    IF(I1+I2+I3+J1+J2+J3)10,10,50
 10 MN=MN+1
    EEE=1.0
    COR=0.0
    GO TO(55,630),MN
 50 IF(M1)11,20,11
 11 IF(M2)12,20,12
 12 IF(M3)13,20,13
 13 IF(N1)14,20,14
 14 IF(N2)15,20,15
 15 IF(N3)17,20,17
 17 IF(L1)18,20,18
 18 IF(L2)19,20,19
 19 IF(L3)25,20,25
 20 EEE=1.0
    COR=0.0
    GO TO 55
 25 EEE=SQRTF((E(I1,I2,I3)+1.0)*(E(J1,J2,J3)+1.0)*(E(K1,K2,K3)+1.0))
    COR=(E(I1,I2,I3)+E(J1,J2,J3)+E(K1,K2,K3)+1.0)/SQRTF(AN)
C   CALCULATE TRIPLE AVERAGES
 55 RN=0.0
    TP=0.0
    DO 600 I=1,IM
    DO 600 J=1,JM
    DO 600 K=1,KM
    IF(E(I,J,K)-B)90,600,90
 90 L=I
    M=J
    N=K
    NNN=0
100 IH=XABSF(L1+L)
    IK=XABSF(L2+M)
    IL=XABSF(L3+N)
    IF(IH)110,500,110
110 IF(IM-IH)500,120,120
120 IF(IK)130,500,130
130 IF(JM-IK)500,140,140
140 IF(IL)150,500,150
150 IF(KM-IL)500,160,160
160 IF(E(IH,IK,IL)-B)165,500,165
165 KH=XABSF(M1+L)
    KK=XABSF(M2+M)
    KL=XABSF(M3+N)
```

```
  167 IF(KH)170,500,170
  170 IF(IM-KH)500,180,180
  180 IF(KK)190,500,190
  190 IF(JM-KK)500,200,200
  200 IF(KL)210,500,210
  210 IF(KM-KL)500,220,220
  220 IF(E(KH,KK,KL)-B)230,500,230
  230 RN=RN+1.0
      TP=TP+E(I,J,K)*E(IH,IK,IL)*E(KH,KK,KL)
  500 NNN=NNN+1
      GO TO(510,520,510,530,510,540,510,600),NNN
  510 L=-L
      M=-M
      N=-N
      GO TO 100
  520 L=-L
      GO TO 100
  530 M=-M
      GO TO 100
  540 M=-M
      N=-N
      GO TO 100
  600 CONTINUE
      TP=TP*SF/RN+COR
      NR=RN
      TPC=TP/EEE
      IF(XMODF(JJJ,15)-1)620,610,620
  610 WRITE OUTPUT TAPE JTP,1100
  620 IF(MN)625,625,621
  621 WRITE OUTPUT TAPE JTP,1300,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
      PRINT 1300,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
      GO TO 9
  625 IF(SENSE SWITCH 1)626,627
  626 PRINT 1200,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
  627 L1=-L1
      L2=-L2
      L3=-L3
      WRITE OUTPUT TAPE JTP,1400,L1,L2,L3
      WRITE OUTPUT TAPE JTP,1200,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
      GO TO 9
  630 CALL EXIT
 1100 FORMAT(1H1,10X,75H  H   K   L    H   K   L    NO.CONTR.   TRIP.PRO
     1D.    COS(INV.)    COR.TERM///)
 1200 FORMAT(1H0,10X,I3,2I4,I5,2I4,3X,I8,2X,3(3X,F10.5))
 1300 FORMAT(1H0,10X,I3,2I4,I5,2I4,3X,I8,2X,3(3X,E10.4))
 1400 FORMAT(1H0,10X,I3,2I4)
      END
```

Triple Product Summation, Noncentrosymmetric

```
CORTHTP  ORTHORHOMBIC TRIP. PROD. PROG.  FOR NONCENTRO. CRYST.
      DIMENSION E(30,10,30)
      ITP=5
      JTP=6
      KTP=9
      REWIND KTP
      B=1.0E-21
      READ INPUT TAPE ITP,1000,NA,IM,JM,KM
 1000 FORMAT(6I10)
      DO 75 I=1,IM
      DO 75 J=1,JM
      DO 75 K=1,KM
   75 E(I,J,K)=B
      READ INPUT TAPE KTP,2000,NOIB
```

```
2000 FORMAT(I7)
     DO 8 NO=1,NOIB
     READ INPUT TAPE KTP,2100,I,J,K,A
2100 FORMAT(3I4,F20.5)
     IF(I)1,8,2
   1 I=-I
   2 IF(J)3,8,4
   3 J=-J
   4 IF(K)5,8,6
   5 K=-K
   6 E(I,J,K)=A
   8 CONTINUE
     REWIND KTP
     AN=NA
     SF=SQRTF(AN**3)/2.0
     JJJ=0
     MN=0
C    START NEW TP CALC.
   9 READ INPUT TAPE ITP,1000,M1,M2,M3,N1,N2,N3
     JJJ=JJJ+1
     I1=XABSF(M1)
     I2=XABSF(M2)
     I3=XABSF(M3)
     J1=XABSF(N1)
     J2=XABSF(N2)
     J3=XABSF(N3)
     L1=M1+N1
     L2=M2+N2
     L3=M3+N3
     K1=XABSF(L1)
     K2=XABSF(L2)
     K3=XABSF(L3)
     IF(I1+I2+I3+J1+J2+J3)10,10,50
  10 MN=MN+1
     EEE=1.0
     COR=0.0
     GO TO(55,630),MN
  50 IF(M1)11,20,11
  11 IF(M2)12,20,12
  12 IF(M3)13,20,13
  13 IF(N1)14,20,14
  14 IF(N2)15,20,15
  15 IF(N3)17,20,17
  17 IF(L1)18,20,18
  18 IF(L2)19,20,19
  19 IF(L3)25,20,25
  20 EEE=1.0
     COR=0.0
     GO TO 55
  25 EEE=SQRTF((E(I1,I2,I3)+1.0)*(E(J1,J2,J3)+1.0)*(E(K1,K2,K3)+1.0))
     COR=(E(I1,I2,I3)+E(J1,J2,J3)+E(K1,K2,K3)+1.0)/SQRTF(AN)
C    CALCULATE TRIPLE AVERAGES
  55 RN=0.0
     TP=0.0
     DO 600 I=1,IM
     DO 600 J=1,JM
     DO 600 K=1,KM
     IF(E(I,J,K)-8)90,600,90
  90 L=I
     M=J
     N=K
     NNN=0
 100 IH=XABSF(L1+L)
     IK=XABSF(L2+M)
     IL=XABSF(L3+N)
     IF(IH)110,500,110
```

```
 110 IF(IM-IH)500,120,120
 120 IF(IK)130,500,130
 130 IF(JM-IK)500,140,140
 140 IF(IL)150,500,150
 150 IF(KM-IL)500,160,160
 160 IF(E(IH,IK,IL)-B)165,500,165
 165 KH=XABSF(M1+L)
     KK=XABSF(M2+M)
     KL=XABSF(M3+N)
 167 IF(KH)170,500,170
 170 IF(IM-KH)500,180,180
 180 IF(KK)190,500,190
 190 IF(JM-KK)500,200,200
 200 IF(KL)210,500,210
 210 IF(KM-KL)500,220,220
 220 IF(E(KH,KK,KL)-B)230,500,230
 230 RN=RN+1.0
     TP=TP+E(I,J,K)*E(IH,IK,IL)*E(KH,KK,KL)
 500 NNN=NNN+1
     GO TO(510,520,510,530,510,540,510,600),NNN
 510 L=-L
     M=-M
     N=-N
     GO TO 100
 520 L=-L
     GO TO 100
 530 M=-M
     GO TO 100
 540 M=-M
     N=-N
     GO TO 100
 600 CONTINUE
     TP=TP*SF/RN+COR
     NR=RN
     TPC=TP/EEE
     IF(XMODF(JJJ,20)-1)620,610,620
 610 WRITE OUTPUT TAPE JTP,1100
 620 IF(MN)625,625,621
 621 WRITE OUTPUT TAPE JTP,1300,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
     PRINT 1300,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
     GO TO 9
 625 WRITE OUTPUT TAPE JTP,1200,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
     PRINT 1200,M1,M2,M3,N1,N2,N3,NR,TP,TPC,COR
     GO TO 9
 630 CALL EXIT
1100 FORMAT(1H1,10X,75H  H   K   L    H   K   L    NO.CONTR.   TRIP.PRO
    1D.    COS(INV.)    COR.TERM///)
1200 FORMAT(1H0,10X,I3,2I4,I5,2I4,3X,I8,2X,3(3X,F10.5))
1300 FORMAT(1H0,10X,I3,2I4,I5,2I4,3X,I8,2X,3(3X,E10.4))
     END
```

Structure Factor Calculation

```
CSTRFAC         STRUCTURE FACTOR EXECUTIVE PROGRAM
     DIMENSION NAME(12),X(3,500),H(3,128),   F1(20),FA1(20),FB(20),FB1(
    1 20),FC(20),       AA(3,3),IA(500),TB(500),AF(500),AF1(500),BF(500
    2 ),BF1(500),CF(500),SI(128),E(128),F(128),A(128),FA(128),P(500),
    3 GYP(500),FK(128),C(128),SF(128),EN(128),B(128),D(128),DF(128),DE(
    4 128),CO(128),DO(128),DC(128),DD(128),AO(128),BO(128),DA(128),DB(I
    5 28),NME(12),FJ(128),AB(3,3),SCF2(100)
```

```
 50 KT=10
    IT=5
    JT=6
    LT=11
    REWIND KT
    REWIND LT
    NASP=0
    I=0
    READ INPUT TAPE IT,1000,(NAME(I),I=1,12)
    READ INPUT TAPE IT,1100,IC,IE,NR,NF,IP,LIB,LINE
    READ INPUT TAPE IT,1200,A1,A2,A3,AL,BE,GA
    READ INPUT TAPE IT,1300,BT,XT,SCF,KKT,IOUT
 60 I=I+1
    READ INPUT TAPE IT,1600,SCF2(I)
    IF(SCF2(I))60,100,60
100 NASP=NASP+1
    READ INPUT TAPE IT,1400,F1(NASP),FA1(NASP),FB(NASP),FB1(NASP),
   1  FC(NASP)
    IF(F1(NASP))100,110,100
110 K=0
120 K=K+1
    READ INPUT TAPE IT,1500,X(1,K),X(2,K),X(3,K),TB(K),IA(K)
    IF(ABSF(X(1,K))+ABSF(X(2,K))+ABSF(X(3,K)))130,130,120
130 K=K-1
    NC=K
140 READ INPUT TAPE IT,1600,T1,T2,T3,U1,U2,U3
    IF(ABSF(T1)+ABSF(T2)+ABSF(T3)+ABSF(U1)+ABSF(U2)+ABSF(U3))170,170,
   1 150
150 DO 160 I=1,NC
    K=K+1
    X(1,K)=T1+U1*X(1,I)
    X(2,K)=T2+U2*X(2,I)
    X(3,K)=T3+U3*X(3,I)
    IA(K)=IA(I)
160 TB(K)=TB(I)
    GO TO 140
170 SDF=0.0
    SFO=0.0
    SDFO=0.0
    DO 180 I=1,K
    J=IA(I)
    AF(I)=F1(J)
    AF1(I)=FA1(J)
    BF(I)=FB(J)
    BF1(I)=FB1(J)
180 CF(I)=FC(J)
    IF(IE)190,195,190
190 NN=1
    GO TO 200
195 NN=2
200 CALL RECIP(A1,A2,A3,AL,BE,GA,AB(1,1),AB(2,2),AB(3,3),AB(2,3),AB(1,
   1 3),AB(1,2))
    DO 230 I=1,3
    DO 230 J=I,3
    IF(I-J)220,210,220
210 AA(I,I)= AB(I,I)**2
    GO TO 230
220 AA(I,J)= 2.0*AB(I,J)*AB(I,I)*AB(J,J)
230 CONTINUE
    IF(NF)240,240,231
231 DO 232 I=1,NF
232 CALL FLSKPD(KT)
240 IF(LIB)242,243,242
242 READ INPUT TAPE KT,1000,(NME(I),I=1,12)
243 GO TO(244,2401),NN
```

```
 244 IF(LINE)2403,2402,2403
2402 READ INPUT TAPE KT,2100,NR
     GO TO 2401
2403 READ INPUT TAPE IT,2100,NR
2401 NO=0
     N1=NR/128
 245 IF(N1-NO)470,250,260
 250 N2=NR-N1*128
     IF(N2)470,470,270
 260 N2=128
 270 GO TO(280,310 ),NN
 280 IF(LINE)281,282,281
 281 READ INPUT TAPE IT,1700,(H(1,I),H(2,I),H(3,I),E(I),I=1,N2)
     GO TO 283
 282 READ INPUT TAPE KT,1700,(H(1,I),H(2,I),H(3,I),E(I),I=1,N2)
 283 DO 300 I=1,N2
     E(I)= SQRTF(E(I)+1.0)*SCF
     SI(I)=0.0
     DO 290L=1,3
     DO 290M=L,3
 290 SI(I)=H(L,I)*H(M,I)*AA(L,M)+SI(I)
 300 SI(I)=SI(I)/4.0
     GO TO 330
 310 IF(LINE)311,312,311
 311 DO 2311 I=1,N2
     READ INPUT TAPE IT,1800, H(1,I),H(2,I),H(3,I),F(I),SCF,SI(I)
     IF(SCF)2314,2314,2313
2313 JK=INTG(SCF)
2314 F(I)=SQRTF(F(I))*SCF2(JK)
2311 CONTINUE
     GO TO 313
 312 DO 3311 I=1,N2
     READ INPUT TAPE KT,1800, H(1,I),H(2,I),H(3,I),F(I),SCF,SI(I)
     IF(SCF)3314,3314,3313
3313 JK=INTG(SCF)
3314 F(I)=SQRTF(F(I))*SCF2(JK)
3311 CONTINUE
 313 IF(SI(1))314,314,317
 314 DO 316 I=1,N2
     SI(I)=0.0
     DO 315 L=1,3
     DO 315 M=L,3
 315 SI(I)=H(L,I)*H(M,I)*AA(L,M)+SI(I)
 316 SI(I)=SI(I)/4.0
     GO TO 330
 317 DO 320 I=1,N2
 320 SI(I)= SI(I)**2
 330 DO 450 I=1,N2
     A(I)=0.0
     SIGK=0.0
     FK(I)=0.0
     DO 350 J=1,K
     FA(J)=AF(J)*EXPF(-AF1(J)*SI(I))+BF(J)*EXPF(-BF1(J)*SI(I))+CF(J)
     SIGK= SIGK+FA(J)**2
     FK(I)=FK(I)+(FA(J)*EXPF(-TB(J)*SI(I)))**2
     P(J)=0.0
     DO 340 L=1,3
 340 P(J)=P(J)+H(L,I)*X(L,J)
     P(J)=P(J)*6.2831853
     GYP(J)=FA(J)*EXPF(-TB(J)*SI(I))
 350 A(I)=A(I)+GYP(J)*COSF(P(J))
     FBTX=EXPF((BT*(SI(I))**XT)/2.0)/SQRTF(SIGK)
     FFAX=1.0/SQRTF(FK(I))
     IF(KKT-1)351,352,353
```

```
351 FK(I)=FFAX
    FJ(I)=FBTX
    GO TO 355
352 FK(I)=FFAX
    FJ(I)=FFAX
    GO TO 355
353 FK(I)=FBTX
    FJ(I)=FBTX
355 C(I)=A(I)*FK(I)
    IF(IC)370,360,370
360 SF(I)=    A(I)
    EN(I)=    C(I)
    GO TO 390
370 B(I)=0.0
    DO 380 J=1,K
380 B(I)=B(I)+ GYP(J)*SINF(P(J))
    D(I)=B(I)*FK(I)
    SF(I)=SQRTF(A(I)**2+B(I)**2)
    EN(I)=SF(I)*FK(I)
390 GO TO(400,410),NN
400 F(I)= E(I)/FJ(I)
    GO TO 420
410 E(I)= F(I)*FJ(I)
420 DF(I)=SIGNF(F(I),SF(I))-SF(I)
    SDF=SDF+ABSF(DF(I))
    SFO=SFO+F(I)
    DE(I)=SIGNF(E(I),EN(I))-EN(I)
    IF(F(I))422,423,422
422 SDFO=SDFO+ABSF(DF(I))
423 IF(IC)425,424,425
424 F(I)=SIGNF(F(I),SF(I))
    E(I)=SIGNF(E(I),EN(I))
    GO TO 450
425 IF(IP)440,430,440
430 TAR=E(I)/ABSF(EN(I))
    CO(I)=C(I)*TAR
    DO(I)=D(I)*TAR
    DC(I)=SIGNF(CO(I),C(I))-C(I)
    DD(I)=SIGNF(DO(I),D(I))-D(I)
    GO TO 450
440 RAT=F(I)/ABSF(SF(I))
    AO(I)=A(I)*RAT
    BO(I)=B(I)*RAT
    DA(I)=SIGNF(AO(I),A(I))-A(I)
    DB(I)=SIGNF(BO(I),B(I))-B(I)
450 CONTINUE
460 IF(IOUT)62,465,62
 62 IF(IC)66,65,66
 65 WRITE OUTPUT TAPE LT,1200,(H(1,I),H(2,I),H(3,I),F(I),E(I),DF(I),
   1DE(I),I=1,N2)
    GO TO 465
 66 IF(IP)68,67,68
 67 WRITE OUTPUT TAPE LT,1200,(H(1,I),H(2,I),H(3,I),CO(I),DO(I),DC(I),
   1DD(I),I=1,N2)
    GO TO 465
 68 WRITE OUTPUT TAPE LT,1200,(H(1,I),H(2,I),H(3,I),AO(I),BO(I),DA(I),
   1DB(I),I=1,N2)
465 CALL OUTSFC(N2,IC,H,F,SF,A,B,E,EN,C,D,DF,NO,AO,BO,DA,DB,CO,DO,DC,
   1 DD,NAME,IP,DE)
    NO=NO+1
    GO TO 245
```

```
 470 REWIND KT
     END FILE LT
     REWIND LT
     R=SDF/SFO
     R1=SDFO/SFO
     WRITE OUTPUT TAPE JT,1900,SFO,SDF,SDFO,R,R1
     READ INPUT TAPE IT,2100,IIJJ
     IF(IIJJ)50,480,50
 480 PRINT 2000
     CALL EXIT
1000 FORMAT(12A6)
1100 FORMAT(7I10)
1200 FORMAT(7F10.4)
1300 FORMAT(3E10.4,2I10)
1400 FORMAT(5F8.4)
1500 FORMAT(4E10.4,I10)
1600 FORMAT(6E10.4)
1700 FORMAT(3F4.0,F20.5)
1800 FORMAT(4F9.2,9X,F9.2,F9.6)
1900 FORMAT(1H1,9X,12HSIGMA F(0) =,F15.3,8X,15HSIGMA /DEL F/ =,F10.3,8X
    1,15HSIGMA /DEL F/ =,F10.3,1H*///24X,2(3HR =,F9.5,9X),1H*////20X,64
    2H* THESE QUANTITIES DO NOT INCLUDE CONTRIBUTIONS FROM REFLECTIONS/
    320X,33H  OBSERVED WITH ZERO INTENSITIES.)
2000 FORMAT(1H1,10X,21HTHIS JOB IS FINISHED.////////////)
2100 FORMAT(I7)
     END
```

Subroutine OUTSFC

```
     SUBROUTINE OUTSFC(N2,IC,H,F,SF,A,B,E,EN,C,D,DF,NO,AO,BO,DA,DB,CO,
    1 DO,DC,DD,NAME,IP,DE)
     DIMENSION H(3,128),F(128),A(128),B(128),E(128),EN(128),C(128),D(12
    1 8),       DF(128),AO(128),BO(128),DA(128),DB(128),CO(128),DO(128)
    2 ,DC(128),DD(128),NAME(12),DE(128),M(3,128),SF(128)
     JT=6
     N4=6*NO
     DO 50  I=1,N2
     DO 50  J=1,3
  50 M(J,I)=INTG(H(J,I))
     IF(128-N2)110,110,100
 100 N1=N2/22
     N3=N2-N1*22
     IF(N1)165,165,120
 110 N1=5
     N3=18
 120 DO 160 I=1,N1
     N4=N4+1
     J1=(I-1)*22+1
     J2=J1+21
     WRITE OUTPUT TAPE JT,1000,(NAME(K),K=1,12),N4
     IF(IC)125,150,125
 125 IF(IP)140,130,140
 130 WRITE OUTPUT TAPE JT,1200
     WRITE OUTPUT TAPE JT,1400,(M(1,J),M(2,J),M(3,J),F(J),SF(J),E(J),
    1 EN(J),CO(J),DO(J),C(J),D(J),DC(J),DD(J),DE(J),J=J1,J2)
     GO TO 160
 140 WRITE OUTPUT TAPE JT,1100
     WRITE OUTPUT TAPE JT,1300,(M(1,J),M(2,J),M(3,J),E(J),EN(J),F(J),
    1 SF(J),AO(J),BO(J),A(J),B(J),DA(J),DB(J),DF(J),J=J1,J2)
     GO TO 160
 150 WRITE OUTPUT TAPE JT,1500
     WRITE OUTPUT TAPE JT,1600,(M(1,J),M(2,J),M(3,J),F(J),SF(J),E(J),
    1 EN(J),DF(J),DE(J),J=J1,J2)
 160 CONTINUE
```

```
 165 IF(N3)210,210,170
 170 J1=N1*22+1
     N4=N4+1
     WRITE OUTPUT TAPE JT,1000,(NAME(K),K=1,12),N4
     IF(IC)175,200,175
 175 IF(IP)190,180,190
 180 WRITE OUTPUT TAPE JT,1200
     WRITE OUTPUT TAPE JT,1400,(M(1,J),M(2,J),M(3,J),F(J),SF(J),E(J),
    1 EN(J),CO(J),DO(J),C(J),D(J),DC(J),DD(J),DE(J),J=J1,N2)
     GO TO 210
 190 WRITE OUTPUT TAPE JT,1100
     WRITE OUTPUT TAPE JT,1300,(M(1,J),M(2,J),M(3,J),E(J),EN(J),F(J),
    1 SF(J),AO(J),BO(J),A(J),B(J),DA(J),DB(J),DF(J),J=J1,N2)
     GO TO 210
 200 WRITE OUTPUT TAPE JT,1500
     WRITE OUTPUT TAPE JT,1600,(M(1,J),M(2,J),M(3,J),F(J),SF(J),E(J),
    1 EN(J),DF(J),DE(J),J=J1,N2)
 210 RETURN
1000 FORMAT(1H1,12A6//100X,4HPAGE,I4/)
1100 FORMAT(120H0  H  K  L      E(O)       E(C)       F(O)       F(C)
    1A(O)       B(O)       A(C)       B(C)      DEL A      DEL B      DEL F /
    2)
1200 FORMAT(120H0  H  K  L      F(O)       F(C)       E(O)       E(C)
    1C(O)       D(O)       C(C)       D(C)      DEL C      DEL D      DEL E /
    2)
1300 FORMAT(1H0,3I3,2F10.4,9F10.3)
1400 FORMAT(1H0,3I3,2F10.3,9F10.4)
1500 FORMAT(86H0     H   K   L         F(O)         F(C)         E(O)
    1 E(C)        DEL F        DEL E /)
1600 FORMAT(2H0 ,3I4,2F12.3,2F12.4,F12.3,F12.4)
     END
```

Interatomic Distance and Angle

```
CBNDANG   BOND DISTANCE AND ANGLE PROGRAM
     DIMENSION NAME(12),N(500),X(500),Y(500),                          02693
    1Z(500),NS1(200),NS2(200),SV(200),N1(2900),N2(2900),
    2D(2900),E1(2900),E2(2900),E3(2900),ANG(2000),
    3M1(2000),M2(2000),M3(2000)                                        02693
     COMMON N1,N2,D,E1,E2,E3
     EQUIVALENCE(M1,N),(M2,X),(M3,Y),(ANG,Z)                           02693
     COSDF(X)=COSF(3.14159*X/180.)
     ITP=5
     JTP=6
     KTP=9
     REWIND KTP
     READ INPUT TAPE ITP,1000,(NAME(II),II=1,12)
     READ INPUT TAPE ITP,1200,A,B,C,AL,BE,GA
     READ INPUT TAPE ITP,1500,BMX,AMX
     READ INPUT TAPE ITP,1100,XINC,YINC,ZINC
     BMX=BMX**2
     CAL=COSDF(AL)
     CBE=COSDF(BE)                                                     02693
     CGA=COSDF(GA)                                                     02693
     I=0                                                               02693
     IF(XINC+YINC+ZINC)107,100,107
 100 I=I+1                                                             02693
     READ INPUT TAPE ITP,1100,X(I),Y(I),Z(I)
 105 N(I)=I-1                                                          02693
     IF(ABSF(X(I))+ABSF(Y(I))+ABSF(Z(I)))110,110,100                   02693
 107 CALL INTERP(I,N,X,Y,Z,ITP,XINC,YINC,ZINC,A,B,C,CAL,CBE,CGA)
```

```
110 JJ=0                                                                02693
    KK=0                                                                02693
    I=I-1
    I1=I                                                                02693
115 READ INPUT TAPE ITP,1200,T1,T2,T3,U1,U2,U3
    IF(ABSF(T1)+ABSF(T2)+ABSF(T3)+ABSF(U1)+ABSF(U2)+ABSF(U3))140,140,   02691
   1 120                                                                02691
120 DO 130 J=1,I                                                        02693
    I1=I1+1                                                             02693
    N(I1)=I1-1                                                          02693
    X(I1)=T1+U1*X(J)                                                    02691
    Y(I1)=T2+U2*Y(J)                                                    02691
130 Z(I1)=T3+U3*Z(J)                                                    02691
    GO TO 115                                                           02693
140 DO 145 J=1,I1
    IF(XMODF(J,50)-1)142,141,142
141 WRITE OUTPUT TAPE JTP,1800,(NAME(K),K=1,12)
142 L1=N(J)/I
    L2=N(J)-L1*I+1
145 WRITE OUTPUT TAPE JTP,1700,L1,L2,X(J),Y(J),Z(J)
150 DO190 J=1,I1                                                        02691
    I2=J+1                                                              02693
    DO 190 K=I2,I1                                                      02693
    IF(N(J)/I-N(K)/I)157,155,157
155 IF(N(J)/I)190,157,190
157 V1=X(J)-X(K)                                                        02693
    V2=Y(J)-Y(K)                                                        02693
    V3=Z(J)-Z(K)                                                        02693
    VEC=ABSF(DOTPRD(V1,V2,V3,V1,V2,V3,A,B,                              02693
   1C,CAL,CBE,CGA))                                                     02693
    IF(VEC- BMX)160,160,190
160 IF(VEC-.49)170,180,180                                              02693
170 JJ=JJ+1                                                             02693
    NS1(JJ)=N(J)                                                        02693
    NS2(JJ)=N(K)                                                        02693
    SV(JJ)=SQRTF(VEC)                                                   02693
    GO TO 190                                                           02693
180 KK=KK+1                                                             02693
    N1(KK)=N(J)                                                         02693
    N2(KK)=N(K)                                                         02693
    D(KK)=SQRTF(VEC)                                                    02693
    E1(KK)=V1                                                           02693
    E2(KK)=V2                                                           02693
    E3(KK)=V3                                                           02693
    IF(2900-KK)330,330,190
190 CONTINUE                                                            02693
    LL=0                                                                02693
    NM=0
    DO 322 J=1,KK
    IF(D(J)-AMX)195,195,322
195 KK1=J+1                                                             02693
    DO 320 K=KK1,KK                                                     02693
    IF(D(K)-AMX)200,200,320
200 IF(N1(J)-N1(K))220,210,220                                          02693
210 M=1.                                                                02693
    ZD=1.0
    GO TO 276
220 IF(N1(J)-N2(K))240,230,240                                          02693
230 M=2                                                                 02693
    ZD=-1.0
    GO TO 276
240 IF(N2(J)-N1(K))260,250,260                                          02693
250 M=3                                                                 02693
    ZD=-1.0
    GO TO 276
```

```
 260 IF(N2(J)-N2(K))320,270,320                                          02693
 270 M=4                                                                 02693
     ZD=1.0
 276 LL=LL+1
     COANG=ZD*  DOTPRD(E1(J),E2(J),E3(J),E1(K),
    1E2(K),E3(K),A,B,C,CAL,CBE,CGA)/(D(J)*D(K))
     ANGCO=1.0-ABSF(COANG)
     IF(ANGCO)2277,277,277
2277 WRITE OUTPUT TAPE  JTP, 1600,N1(J),N2(J),N1(K),N2(K),ANGCO
     COANG=1.0
 277 ANG(LL)=90.00-57.295780*ARCSIN(COANG)
 278 GO TO(280,290,300,310),M                                            02693
 280 M1(LL)=N2(J)                                                        02693
     M2(LL)=N1(J)                                                        02693
     M3(LL)=N2(K)                                                        02693
     GO TO 315
 290 M1(LL)=N2(J)                                                        02693
     M2(LL)=N1(J)                                                        02693
     M3(LL)=N1(K)                                                        02693
     GO TO 315
 300 M1(LL)=N1(J)                                                        02693
     M2(LL)=N2(J)                                                        02693
     M3(LL)=N2(K)                                                        02693
     GO TO 315
 310 M1(LL)=N1(J)                                                        02693
     M2(LL)=N2(J)                                                        02693
     M3(LL)=N1(K)                                                        02693
 315 IF(2000-LL)360,360,320
 360 WRITE TAPE KTP,(M1(MN),M2(MN),M3(MN),ANG(MN),MN=1,2000)
     LL=0
     NM=NM+1
 320 CONTINUE                                                            02693
 322 CONTINUE
     IF(LL)323,323,1323
1323 WRITE TAPE KTP,(M1(MN),M2(MN),M3(MN),ANG(MN),MN=1,LL)
 323 CALL OUTBND(I,JJ,KK,LL,NS1,NS2,SV,                                  02693
    1N1,N2,N3,D,E1,E2,E3,ANG,M1,M2,M3,                                   02693
    2NAME,JTP,NM,KTP)
 325 CALL EXIT
 330 BMX=(SQRTF(BMX)-.25)**2
     IF(BMX-4.0)335,335,370
 335 IF(I1/I-1)340,340,350
 340 WRITE OUTPUT TAPE JTP,1300
     GO TO 325
 350 WRITE OUTPUT TAPE JTP,1400
     I1=I                                                                02691
 370 KK=0
     JJ=0
     GO TO 150                                                           02691
1000 FORMAT(12A6)                                                        02693
1100 FORMAT(3E10.4)                                                      02693
1200 FORMAT(6E10.4)                                                      02693
1300 FORMAT(1H1,8X,71HMORE THAN 2900  2 A. OR LESS BOND DISTANCES   HAV
    1E BEEN FOUND AMONG THE///9X,71HUNTRANSLATED SET OF ATOMS.  THIS PR02691
    2OBLEM IS TOO LARGE.  NO RESULTS WILL///9X,10HBE ISSUED.)           02691
1400 FORMAT(1H1,8X,71HMORE THAN 2900  2 A. OR LESS BOND DISTANCES   HAV
    1E BEEN FOUND.  VECTORS///9X,58HWILL BE CONSIDERED FOR THE UNTRANSL02691
    2ATED SET OF ATOMS ONLY.)                                            02691
1500 FORMAT(2E10.4)
1600 FORMAT(10X,4I4,E12.5)
1700 FORMAT(11X,I2,1H-,I2,3F10.5)
1800 FORMAT(1H1,10X,12A6///12X,4HATOM,6X,1HX,9X,1HY,9X,1HZ/)
     END
```

Subroutine INTERP

```
      SUBROUTINE INTERP(I,N,X,Y,Z,ITP,XINC,YINC,ZINC,A,B,C,CAL,CBE,CGA)
      DIMENSION X(500),Y(500),Z(500),N(500),P(7),E(3,3),G(3,4),H(3)
      E(1,1)=1.0
      E(1,2)=B*CGA*YINC/(XINC*A)
      E(1,3)=C*CBE*ZINC/(XINC*A)
      E(2,1)=A*CGA*XINC/(YINC*B)
      E(2,2)=1.0
      E(2,3)=C*CAL*ZINC/(YINC*B)
      E(3,1)=A*CBE*XINC/(ZINC*C)
      E(3,2)=B*CAL*YINC/(ZINC*C)
      E(3,3)=1.0
  100 I=I+1
      READ INPUT TAPE ITP,1000,X(I),Y(I),Z(I)
      IF(ABSF(X(I))+ABSF(Y(I))+ABSF(Z(I)))130,130,110
  110 READ INPUT TAPE ITP,1000,(P(J),J=1,7)
      L=0
      DO 120 J=1,3
      L=L+2
      G(J,4)=LOGF(P(1)/P(L))/LOGF(P(1)/P(L+1))
      G(J,4)=(G(J,4)-1.0)/(2.0*(G(J,4)+1.0))
      DO 120 K=1,3
  120 G(J,K)=E(J,K)
      CALL MATS(G,H,3,1)
      X(I)=X(I)+H(1)*XINC
      Y(I)=Y(I)+H(2)*YINC
      Z(I)=Z(I)+H(3)*ZINC
      N(I)=I-1
      GO TO 100
  130 RETURN
 1000 FORMAT(7E10.4)
      END
```

Subroutine OUTBND

```
      SUBROUTINE OUTBND(I,JJ,KK,LM,NS1,
     1NS2,SV,N1,N2,N3,D,E1,E2,E3,ANG,M1,
     2M2,M3,NAME,JTP,NM,KTP)
C     OUTPUT S.R. FOR BOND DISTANCE AND ANGLE PROGRAM                    02693
      DIMENSION NS1(200),NS2(200),SV(200),                              02693
     1N1(3000),N2(3000),D(3000),E1(3000),E2(3000),
     2E3(3000),ANG(2000),M1(2000),M2(2000),
     3M3(2000),NAME(12)                                                 02693
      REWIND KTP
      IJK=1                                                             02693
   50 I1=KK/44                                                          02693
      IF(KK)85,85,75                                                    02693
   75 IF(I1)120,120,100                                                 02693
   85 WRITE OUTPUT TAPE JTP,8000
      GO TO 250                                                         02693
  100 DO 110 J=1,I1                                                     02693
      WRITE OUTPUT TAPE JTP,1000,(NAME(K),K=1,12),J
      I3=J*44-22                                                        02693
      I2=I3-21
      DO 110 L=I2,I3                                                    02693
      L1=N1(L)/I                                                        02693
      M11=N1(L)-L1*I+1                                                  02693
      L2=N2(L)/I                                                        02693
      M22=N2(L)-L2*I+1                                                  02693
      LL1=N1(L+22)/I                                                    02693
      MM1=N1(L+22)-LL1*I +1                                             02693
      LL2=N2(L+22)/I                                                    02693
      MM2=N2(L+22)-LL2*I +1                                             02693
```

```
110 WRITE OUTPUT TAPE JTP,2000,L1,M11,L2,M22,D(L),LL1,MM1,LL2,MM2,
   1D(L+22)
    IF(KK-I1*44)170,170,120                                    02693
120 I4=I1*44+1                                                 02693
    I5=KK-I4-21                                                02693
    IF(I5)121,122,122
121 I5=0
122 I6=I4+I5-1
    I7=I6+1
    I8=KK-I5
    I9=I1+1                                                    02693
    WRITE OUTPUT TAPE JTP,1000,(NAME(K),K=1,12),I9
    IF(I5)150,150,130                                          02693
130 DO140 L=I4,I6                                              02693
    L1=N1(L)/I                                                 02693
    M11=N1(L)-L1*I +1                                          02693
    L2=N2(L)/I                                                 02693
    M22=N2(L)-L2*I+1
    LL1=N1(L+22)/I
    MM1=N1(L+22)-LL1*I +1                                      02693
    LL2=N2(L+22)/I                                             02693
    MM2=N2(L+22)-LL2*I +1                                      02693
140 WRITE OUTPUT TAPE JTP,2000,L1,M11,L2,M22,D(L),LL1,MM1,
   1LL2,MM2,D(L+22)                                            02693
150 DO 160 L=I7,I8                                             02693
    L1=N1(L)/I                                                 02693
    M11=N1(L)-L1*I +1                                          02693
    L2=N2(L)/I                                                 02693
    M22=N2(L)-L2*I +1                                          02693
160 WRITE OUTPUT TAPE JTP,3000,L1,M11,L2,M22,D(L)
170 GO TO(175,270),IJK                                         02693
175 IF(NM)250,1176,1175
1175 LL=2000
    GO TO 1177
1176 LL=LM
    IF(LL)250,250,1177
1177 NM=NM-1
    READ TAPE KTP,(M1(MN),M2(MN),M3(MN),ANG(MN),MN=1,LL)
    J1=LL/44
176 IF(J1)200,200,180                                          02693
180 DO 190 K=1,J1
    WRITE OUTPUT TAPE JTP,4000,(NAME(L),L=1,12),K
    J3=K*44-22                                                 02693
    J2=J3-21
    DO 190 N=J2,J3                                             02693
    L1=M1(N)/I                                                 02693
    L2=M1(N)-L1*I +1                                           02693
    L3=M2(N)/I                                                 02693
    L4=M2(N)-L3*I +1                                           02693
    L5=M3(N)/I                                                 02693
    L6=M3(N)-L5*I +1                                           02693
    ML1=M1(N+22)/I                                             02693
    ML2=M1(N+22)-ML1*I +1                                      02693
    ML3=M2(N+22)/I                                             02693
    ML4=M2(N+22)-ML3*I +1                                      02693
    ML5=M3(N+22)/I                                             02693
    ML6=M3(N+22)-ML5*I +1                                      02693
190 WRITE OUTPUT TAPE JTP,5000,L1,L2,L3,L4,L5,L6,ANG(N),
   1ML1,ML2,ML3,ML4,ML5,ML6,ANG(N+22)                          02693
    IF(LL-J1*44)175,175,200
200 J4=J1*44+1                                                 02693
    J5=LL-J4-21                                                02693
    IF(J5)201,202,202
201 J5=0
```

```
202 J6=J4+J5-1
    J7=J6+1
    J8=LL-J5
    J9=J1+1                                                          02693
    WRITE OUTPUT TAPE JTP,4000,(NAME(L),L=1,12),J9
    IF(J5)230,230,210                                                02693
210 DO 220 N=J4,J6                                                   02693
    L1=M1(N)/I                                                       02693
    L2=M1(N)-L1*I +1                                                 02693
    L3=M2(N)/I                                                       02693
    L4=M2(N)-L3*I  +1                                                02693
    L5=M3(N)/I                                                       02693
    L6=M3(N)-L5*I +1                                                 02693
    ML1=M1(N+22)/I                                                   02693
    ML2=M1(N+22)-ML1*I  +1                                           02693
    ML3=M2(N+22)/I                                                   02693
    ML4=M2(N+22)-ML3*I  +1                                           02693
    ML5=M3(N+22)/I                                                   02693
    ML6=M3(N+22)-ML5*I +1                                            02693
220 WRITE OUTPUT TAPE JTP,5000,L1,L2,L3,L4,L5,L6,ANG(N),
   1ML1,ML2,ML3,ML4,ML5,ML6,ANG(N+22)                                02693
230 DO 240 N=J7,J8                                                   02693
    L1=M1(N)/I                                                       02693
    L2=M1(N)-L1*I +1                                                 02693
    L3=M2(N)/I                                                       02693
    L4=M2(N)-L3*I  +1                                                02693
    L5=M3(N)/I                                                       02693
    L6=M3(N)-L5*I  +1                                                02693
240 WRITE OUTPUT TAPE JTP,6000,L1,L2,L3,L4,L5,L6,ANG(N)
    GO TO 175
250 IF(JJ)265,265,255                                                02693
255 KK=JJ                                                            02693
    DO 260 J=1,JJ                                                    02693
    N1(J)=NS1(J)                                                     02693
    N2(J)=NS2(J)                                                     02693
260 D(J)=SV(J)                                                       02693
    WRITE OUTPUT TAPE JTP,7000
    IJK=2                                                            02693
    GO TO 50
265 WRITE OUTPUT TAPE JTP,9000
270 REWIND KTP
    RETURN
1000 FORMAT(1H1,6X,30HBOND DISTANCES(ANGSTROMS) FOR ,12A6,7H  PAGE ,I2/02693
   1//19X,24HATOM    ATOM    DISTANCE,27X,24HATOM    ATOM    DISTANCE)02693
2000 FORMAT(1H0,17X,I2,1H-,I2,3X,I2,1H-,I2,4X,F8.5,26X,I2,1H-,I2,3X,I2,
   11H-,I2,4X,F8.5)
3000 FORMAT(1H0,17X,I2,1H-,I2,3X,I2,1H-,I2,4X,F8.5)
4000 FORMAT(1H1,6X,30HBOND ANGLES (DEGREES) FOR     ,12A6,7H  PAGE ,I2/02693
   1//2(11X,32HATOM    ATOM    ATOM       ANGLE,11X))                  02693
5000 FORMAT(1H0,2(9X,I2,1H-,I2,3X,I2,1H-,I2,3X,I2,1H-,I2,4X,F9.4,10X)) 02693
6000 FORMAT(1H0,9X,I2,1H-,I2,3X,I2,1H-,I2,3X,I2,1H-,I2,4X,F9.4)         02693
7000 FORMAT(1H1,10X,53HTHE FOLLOWING BOND DISTANCES ARE ALL LESS THAN 002693
   1.7 A.//11X,59HBOND ANGLES INVOLVING THESE BONDS HAVE NOT BEEN CALC02693
   1ULATED.)                                                         02693
8000 FORMAT(1H1,10X,64HNO BOND DISTANCES BETWEEN 0.7 AND 4.0 ANGSTROMS 02693
   1HAVE BEEN FOUND.)                                                02693
9000 FORMAT(1H1,10X,58HNO BOND DISTANCES LESS THAN 0.7 ANGSTROMS HAVE B02693
   1EEN FOUND.)                                                      02693
    END                                                              02693
```

Least-Squares Line and Plane Fitter

```
CLSQPLN   LEAST-SQUARES LINE AND PLANE FITTER
      DIMENSION ZZ(12),G(3,3),ZY(10),X(3,50),WXS(3), WXXS(3,3),WT(50),
     1ADJ(3,3), A(3,3),G1(3,3),XMK(3),B(3,3),YMK(3),VM(3,3),VMI(3,3),
     2VMJ(3,3), C(3,3), DI(50),DEL(50),DEL2(50),XBAR(3),VMK(3,50),
     3P(3),UMK(3,50) ,BV(3)
     4,Z12(3)
      ITP=5
      JTP=6
      Z34=1.0E-12
      MM=10
      READ INPUT TAPE ITP,1000,(ZZ(I),I=1,12)
      READ INPUT TAPE ITP,1003,A1,A2,A3,AL,BE,GA
      WRITE OUTPUT TAPE JTP,1020,(ZZ(I),I=1,12)
      CALL RECIP(A1,A2,A3,AL,BE,GA,B1,B2,B3,COSA,COSB,COSC)
C     SET UP MATRIX G
      G(1,1)=B1**2
      G(1,2)=B1*B2*COSC
      G(1,3)=B1*B3*COSB
      G(2,1)=G(1,2)
      G(2,2)=B2**2
      G(2,3)=B2*B3*COSA
      G(3,1)=G(1,3)
      G(3,2)=G(2,3)
      G(3,3)=B3**2
      G1(1,1)=A1**2
      G1(1,2)=A1* A2*COSF(GA*3.14159/180.0)
      G1(1,3)=A1*A3*COSF(BE*3.14159/180.0)
      G1(2,1)=G1(1,2)
      G1(2,2)=A2**2
      G1(2,3)=A2*A3*COSF(AL*3.14159/180.0)
      G1(3,1)=G1(1,3)
      G1(3,2)=G1(2,3)
      G1(3,3)=A3**2
      READ INPUT TAPE ITP,1002,N,NO,L,(ZY(I),I=1,10)
   10 DO 20 J=1,N
   20 READ INPUT TAPE ITP,1003, X(1,J),X(2,J),X(3,J),WT(J)
C     COORDINATES OF CENTROID
      DO 25 I=1,N
      IF(WT(I))25,22,25
   22 WT(I)=1.0
   25 CONTINUE
      DO 30 I=1,3
      WXS(I)=0.
      DO 30 J=1,N
   30 WXS(I)=WXS(I)+WT(J)*X(I,J)
      WS=0.
      DO 40 I=1,N
   40 WS=WS+WT(I)
      DO 50 I=1,3
   50 XBAR(I)=WXS(I)/WS
C     SET UP MATRIX A
      DO 60 I=1,3
      DO 60 J=1,3
      WXXS(I,J)=0.
      DO 55 K=1,N
   55 WXXS(I,J)=WXXS(I,J)+WT(K)*X(I,K)*X(J,K)
   60 A(I,J)=WXXS(I,J)-XBAR(I)*XBAR(J)*WS
      IF(L)65,65,61
C    EVALUATE MATRIX B FOR LINE
   61 CALL MTXMUL(3,3,3,G1,A,B)
      GO TO 75
C    SET UP ADJOINT OF A
```

```
   65 ADJ(1,1)=A(2,2)*A(3,3)-A(2,3)*A(3,2)
      ADJ(2,1)=A(3,1)*A(2,3)-A(2,1)*A(3,3)
      ADJ(3,1)=A(2,1)*A(3,2)-A(3,1)*A(2,2)
      ADJ(1,2)=A(3,2)*A(1,3)-A(1,2)*A(3,3)
      ADJ(2,2)=A(1,1)*A(3,3)-A(3,1)*A(1,3)
      ADJ(3,2)=A(3,1)*A(1,2)-A(1,1)*A(3,2)
      ADJ(1,3)=A(1,2)*A(2,3)-A(1,3)*A(2,2)
      ADJ(2,3)=A(2,1)*A(1,3)-A(1,1)*A(2,3)
      ADJ(3,3)=A(1,1)*A(2,2)-A(2,1)*A(1,2)
C     EVALUATE DETERMINANT OF A
      CALL MTXMUL(3,3,3,ADJ,A,C)
      DETNA=0.
      DO 70 I=1,3
   70 DETNA=DETNA+C(I,I)
      DETNA=DETNA/3.0
C     EVALUATE MATRIX B FOR PLANE
      CALL MTXMUL(3,3,3,ADJ,G,B)
   75 DO 80 I=1,3
   80 BV(I)=0.
      DO 90 I=1,3
      DO 90 J=1,3
   90 BV(I)=BV(I)+B(J,I)**2
      BIGBV=BV(1)
      KK=1
      DO 110 I=2,3
      IF(BV(I)-BIGBV)110,110,100
  100 KK=I
      BIGBV=BV(I)
  110 CONTINUE
      VMN=SQRTF(BIGBV)
      DO 120 I=1,3
  120 VM(I,1)=B(I,KK)/VMN
      NNN=0
C     EVALUATE VM BY ITERATION
  125 CALL MTXMUL(3,3,1,B,VM,VMI)
      NNN=NNN+1
      IF(MM-NNN)3,3,4
    3 MM=MM+10
      Z34=Z34*100.
    4 IF(40-NNN)1,1,2
    1 WRITE OUTPUT TAPE JTP,1021,NO
      GO TO 235
    2 IJ=1
      VMN=SQRTF(VMI(1,1)**2+VMI(2,1)**2+VMI(3,1)**2)
      DO 126 I=1,3
  126 VMI(I,1)=VMI(I,1)/VMN
      DO 140 I=1,3
      Z12(I)=VM(I,1)/VMI(I,1)-1.0
      IF(ABSF ((VM(I,1)/VMI(I,1))-1.0)-Z34     )140,140,130
  130 IJ=2
      GO TO 150
  140 CONTINUE
  150 DO 160 I=1,3
      VM(I,1)=VMI(I,1)
  160 VM(1,I)=VM(I,1)
      GO TO(170,125),IJ
C     NORMALIZE VECTOR VM
  170 CALL MTXMUL(1,3,3,VM,G,VMI)
      CALL MTXMUL(1,3,1,VMI,VM,VMJ)
      ORM=SQRTF(VMJ(1,1))
      DO 180 I=1,3
  180 VM(I,1)=VM(I,1)/ORM
      IF(L)185,185,500
```

```
  500 DO 510 I=1,3
      P(I)=0.0
      DO 510 J=1,3
  510 P(I)=VM(J,1)*G(J,I)+P(I)
      DL2=0.0
      DO 530 I=1,N
      DEL2(I)=0.0
      DO 520 J=1,3
      DO 520 K=1,3
  520 DEL2(I)=DEL2(I)+(XBAR(J)-X(J,I))*(XBAR(K)-X(K,I))*(G1(J,K)-
     1VM(J,1)*VM(K,1))
  530 DL2=DL2+DEL2(I)
      WRITE OUTPUT TAPE JTP,1025,NO,N,(ZY(I),I=1,10),XBAR(1),P(1),XBAR(2
     1),P(2),XBAR(3),P(3),(I,WT(I),DEL2(I),I=1,N)
      SATN=N-2
      IF(SATN)550,550,540
  540 STND=SQRTF(DL2/SATN)
      WRITE OUTPUT TAPE JTP,1032,STND
  550 DO 560 I=1,3
  560 UMK(I,NO)=VM(I,1)
      GO TO 235
C     EVALUATE EIGEN VALUE FOR PLANE
  185 CALL MTXMUL(3,3,1,B,VM,VMJ)
      DNEG=0.
      DO 190 I=1,3
  190 DNEG=DNEG+VMJ(I,1)/VM(I,1)
      EIGEN=3.0*DETNA/DNEG
C     EVALUATE D(PLANE TO ORIGIN DISTANCE)
      D=0.
      DO 200 I=1,3
  200 D=D+VM(I,1)*XBAR(I)
C     EVALUATE D,DELTA D,(DELTA D)**2 FOR EACH POINT
      DL2=0.
      DO 220 I=1,N
      DI(I)=0.
      DO 210 J=1,3
  210 DI(I)=DI(I)+VM(J,1)*X(J,I)
      DEL(I)=DI(I)-D
      DEL2(I)=DEL(I)**2
  220 DL2=DL2+WT(I)*DEL2(I)
      DO 230 I=1,3
  230 VMK(I,NO)=VM(I,1)
C     OUTPUT ONE
      WRITE OUTPUT TAPE JTP,1005,NO,N,(ZY(I),I=1,10),VM(1,1),VM(2,1),VM(
     13,1),D,XBAR(1),XBAR(2),XBAR(3),(I,WT(I),DI(I),DEL(I),DEL2(I),I=1,N
     2)
      WRITE OUTPUT TAPE JTP,1012,DL2,EIGEN
      AVED=0.
      DO 231 I=1,N
  231 AVED=AVED+DI(I)
      ATN=N
      AVED=AVED/ATN
      SATN=N-3
      IF(SATN)232,232,233
  232 WRITE OUTPUT TAPE JTP,1018,AVED
      GO TO 235
  233 STND=SQRTF(DL2/SATN)
      WRITE OUTPUT TAPE JTP,1019,AVED,STND
C     INTERROGATE NEXT CARD
  235 READ INPUT TAPE ITP,1002,N,NO,L,(ZY(I),I=1,10)
      IF(N)240,240,10
  240 READ INPUT TAPE ITP,1013,N,L1,NO,L2
      IF(N)270,270,245
C     OUTPUT TWO
```

```
245 WRITE OUTPUT TAPE JTP,1014
    GO TO 260
250 READ INPUT TAPE ITP,1013,N,L1,NO,L2
    IF(N)270,270,260
260 IF(L1)275,275,300
275 IF(L2)280,280,340
280 DO 290 I=1,3
    XMK(I)=VMK(I,N)
290 YMK(I)=VMK(I,NO)
    LLL=1
    GO TO 350
300 IF(L2)310,310,330
310 DO 320 I=1,3
    XMK(I)=UMK(I,N)
320 YMK(I)=VMK(I,NO)
    LLL=2
    GO TO 350
330 DO 335 I=1,3
    XMK(I)=UMK(I,N)
335 YMK(I)=UMK(I,NO)
    LLL=3
    GO TO 350
340 DO 345 I=1,3
    XMK(I)=VMK(I,N)
345 YMK(I)=UMK(I,NO)
    LLL=4
350 DTPD=DOTPRD(XMK(1),XMK(2),XMK(3),YMK(1),YMK(2),YMK(3),B1,B2,B3,
   1COSA,COSB,COSC)
    WRITE OUTPUT TAPE JTP,1006
    GO TO(360,370,380,390),LLL
360 WRITE OUTPUT TAPE JTP,1016,N,NO,DTPD
    GO TO 250
370 WRITE OUTPUT TAPE JTP,1036,N,NO,DTPD
    GO TO 250
380 WRITE OUTPUT TAPE JTP,1035,N,NO,DTPD
    GO TO 250
390 WRITE OUTPUT TAPE JTP,1037,N,NO,DTPD
    GO TO 250
270 PRINT 1017
    CALL EXIT
1000 FORMAT(12A6)
1002 FORMAT(2I3,I6,10A6)
1003 FORMAT(6E10.4)
1005 FORMAT(1H1,7X,12HPLANE NUMBERI4,I10,6H ATOMS,7X,10A6////12X,90HEQU
    2ATION OF PLANE IS     M1*X + M2*Y + M3*Z = D      WHERE D IS THE ORI
    3GIN TO PLANE DISTANCE/1H0,20X,3HM1=E12.5,7H     M2=E12.5,7H     M3=E
    412.5,6H     D=E12.5////12X,32HCOORDINATES OF CENTROID       X =E12.5
    5,5X,3HY =E12.5,5X,3HZ =12.5////15X,72HATOM NUMBER     WEIGHT
    6     D              DELTA D        (DELTA D)**2/(1H0,17X,I3,6X,E10.4,
    75X,E12.5,5X,E12.5,4X,E12.5))
1006 FORMAT(1H0)
1012 FORMAT(////15X,21HSUM WT*(DELTA D)**2 =E12.5,20X,13HEIGEN VALUE =E
    112.5///)
1013 FORMAT(4I3)
1014 FORMAT(1H1,29X,40HDIHEDRAL ANGLES BETWEEN PLANES AND LINES////29X,
    134HANGLE BETWEEN PLANES P1 AND P2 = A/1H0,28X,33HANGLE BETWEEN LIN
    2ES L1 AND L2 = B/1H0,28X,36HANGLE BETWEEN LINE L AND PLANE P = C)
1016 FORMAT(1H0,28X,4HP1 =I3,10H      P2 =I3,17H      COSINE(A) =E12.5)
1017 FORMAT(1H1,9X,13HJOB FINISHED.///////////)
1018 FORMAT(1H0,14X,11HAVERAGE D =E12.5)
1019 FORMAT(1H0,14X,11HAVERAGE D =E12.5,15X,20HSTANDARD DEVIATION =E12.
    15)
1020 FORMAT (1H1,35X,12A6)
1021 FORMAT(1H1,71H     A SATISFACTORY LEAST SQUARES FIT CANNOT BE FOUN
    1D FOR  SET  NUMBER I3,38H.  EXAMINE INPUT PARAMETERS FOR ERROR.)
```

```
1025 FORMAT(1H1,8X,11HLINE NUMBERI4,I10,6H ATOMS,7X,10A6////12X,40HTHE
    1PARAMETRIC EQUATIONS OF THE LINE ARE//37X,4HX = E12.5,5H  +  E12.5
    2,4H * T//37X,4HY = E12.5,5H  +  E12.5,4H * T//37X,4HZ = E12.5,5H
    3+  E12.5,4H * T////12X,46HTHE SQUARE DEVIATIONS FROM THE LINE, D**
    42, ARE//  22X,11HATOM NUMBER,11X,6HWEIGHT,14X,4HD**2/(1HO,24X,I3,1
    54X,E12.5,6X,E12.5))
1032 FORMAT(////12X,21HSTANDARD DEVIATION = E12.5)
1035 FORMAT(1HO,28X,4HL1 =I3,10H       L2 =I3,17H       COSINE(B) =E12.5)
1036 FORMAT(1HO,28X,4H L =I3,10H        P =I3,17H         SINE(C) =E12.5)
1037 FORMAT(1HO,28X,4H P =I3,10H        L =I3,17H         SINE(C) =E12.5)
     END
```

Point to Peak Distance Calculation

```
ATDIST   DETERMINES DISTANCES OF ATOMS FROM ANY POINT IN UNIT CELL

     DIMENSION NAME(12),N(500),X(500),Y(500),
    1Z(500),NS1(200),NS2(200),SV(200),N1(5000),N2(5000),
    2JNT(11),NINT(100,11),AVE(100),EDM(100),NTB(100),D(5000),TT(11),
    3TV(11) ,DIS(11),DISA(100,11)
     COSDF(X)=COSF(3.14159*X/180.)
     ITP=5
     JTP=6
     READ INPUT TAPE ITP,1000,(NAME(II),II=1,12)
     READ INPUT TAPE ITP,1200,A,B,C,AL,BE,GA
     READ INPUT TAPE ITP,1100,BMX
     READ INPUT TAPE ITP, 1100,XC,YC,ZC
     BMX=BMX**2
     I=0
 100 I=I+1
     READ INPUT TAPE ITP,1100,X(I),Y(I),Z(I)
 105 N(I)=I-1
     IF(ABSF(X(I))+ABSF(Y(I))+ABSF(Z(I)))110,110,100
 110 JJ=0
     KK=0
     I=I-1
     I1=I
 115 READ INPUT TAPE ITP,1200,T1,T2,T3,U1,U2,U3
     IF(ABSF(T1)+ABSF(T2)+ABSF(T3)+ABSF(U1)+ABSF(U2)+ABSF(U3))140,140,
    1 120
 120 DO 130 J=1,I
     I1=I1+1
     N(I1)=I1-1
     X(I1)=T1+U1*X(J)
     Y(I1)=T2+U2*Y(J)
 130 Z(I1)=T3+U3*Z(J)
     GO TO 115
 140 CAL=COSDF(AL)
     CBE=COSDF(BE)
     CGA=COSDF(GA)
 150 DO190 J=1,I1
 157 V1=X(J)-XC
     V2=Y(J)-YC
     V3=Z(J)-ZC
     VEC=ABSF(DOTPRD(V1,V2,V3,V1,V2,V3,A,B,
    1C,CAL,CBE,CGA))
     IF(VEC-BMX)180,180,190
 180 KK=KK+1
     N1(KK)=N(J)
     D(KK)=SQRTF(VEC)
```

```
 190 CONTINUE
     WRITE OUTPUT TAPE JTP,3300,(NAME(K),K=1,12)
     DO 200 J=1,KK
     L1=N1(J)/I
     M1=N1(J)-L1*I+1
 200 WRITE OUTPUT TAPE JTP,2000,L1,M1,D(J)
     READ INPUT TAPE ITP, 1100,XC,YC,ZC
     IF(ABSF(XC)+ABSF(YC)+ABSF(ZC))2190,2190,210
 210 KK=0
     GO TO 150
2190 CALL EXIT
1000 FORMAT(12A6)
1100 FORMAT(3E10.4)
1200 FORMAT(6E10.4)
2000 FORMAT(1HO,17X,I2,1H-,I2,4X,F8.5)
3300 FORMAT(1H1,10X,12A6)
     END(1,1,0,0,0,0,1,0,0,0,0,0,0,0,0)
```

Form Factors for Busing Least Squares

```
CFORMBUS  FORM FACTORS FOR BUSING LEAST-SQ. REFIN. PROGRAM
     DIMENSION S(33),F(32),NC(25),BLANK(12)
     ITP=5
     JTP=6
     KT=10
     REWIND KT
     READ INPUT TAPE ITP,250, (BLANK(I),I=1,12)
     NC(1)=1
     NC(9)=2
     NC(17)=3
     NC(25)=4
   5 READ INPUT TAPE ITP,
    1      100,A,A1,B,B1,C,ATOM
     IF(A)30,30,10
  10 S(1)=1.55
     DO 20 I=1,32
     F(I)=A*EXPF(-A1*S(I)**2)+B*EXPF(-B1*S(I)**2)+C
  20 S(I+1)=S(I)-.05
     WRITE OUTPUT TAPE JTP,  200,ATOM
     WRITE OUTPUT TAPE JTP, 210
     WRITE OUTPUT TAPE JTP,   220
     WRITE OUTPUT TAPE JTP,    210
     WRITE OUTPUT TAPE JTP,
    1      230,(S(I),F(I),S(I+16),F(I+16),I=1,16)
     WRITE OUTPUT TAPEKT,250,(BLANK(I),I=1,12)
     WRITE OUTPUT TAPEKT,240,(F(I),F(I+1),F(I+2),F(I+3),F(I+4),
    1F(I+5),F(I+6),F(I+7),ATOM,NC(I),I=1,25,8)
     GO TO 5
  30 END FILE KT
     REWIND KT
     CALL EXIT
 100 FORMAT(5F8.5,A6)
 200 FORMAT(1H1,9X,A6)
 210 FORMAT(1HO)
 220 FORMAT(1HO,9X,7HSIN()/L,13X,11HFORM FACTOR,29X,7HSIN()/L,13X,11HFO
    1RM FACTOR)
 230 FORMAT(1HO,9X,F5.2,15X,F10.6,30X,F5.2,15X,F10.6)
 240 FORMAT(7F9.4,F8.4,1HF,A6,I2)
 250 FORMAT(12A6)
     END
```

Variance-Covariance and Atomic Parameter Input for Busing Function and Error

```
CBUSVAR   VARIANCE MATRIX INPUT FOR BUSING ERROR FUNCTION PROGRAM
      DIMENSION A(18528),B(192)
      ITP=5
      JTP=6
      I5=9
      REWINDI5
      READ INPUT TAPE ITP,
     1     100,N,SF
      READ INPUT TAPE ITP,
     1     200,A1,A2,A3
      DO 10 I=1,N,3
      READ INPUT TAPE ITP,
     1     200,B(I),B(I+1),B(I+2)
    5 B(I)=(B(I)/A1)**2
      B(I+1)=(B(I+1)/A2)**2
   10 B(I+2)=(B(I+2)/A3)**2
      SF=SF**2
      M=0
      DO 40 I=1,N
      DO 40 J=1,N
      IF(I-J)20,30,40
   20 M=M+1
      A(M)=0.0
      GO TO 40
   30 M=M+1
      A(M)=B(I)
   40 CONTINUE
      MN=M/8
      IF(M-8*MN)45,45,41
   41 L=M+1
      M=MN*8+8
      DO 43 I=L,M
   43 A(I)=0.0
   45 IF(SENSESWITCH 1)46,47
   46 MM=1
      PUNCH 600
      PUNCH 100,N,SF
      GO TO 48
   47 MM=2
      WRITE OUTPUT TAPEI5,100,N,SF
   48 K=0
      DO 55 I=1,M,8
      K=K+1
      GO TO(51,50),MM
   50 WRITE OUTPUT TAPEI5,300,A(I),A(I+1),A(I+2),A(I+3),A(I+4),A(I+5),
     1A(I+6),A(I+7),K
      GO TO 55
   51 PUNCH 700,A(I),A(I+1),A(I+2),A(I+3),A(I+4),A(I+5),A(I+6),A(I+7)
   55 CONTINUE
      READ INPUT TAPE ITP,
     1     200,(B(I),B(I+1),B(I+2),I=1,N,3)
      IJ=N/8
      IF(N-IJ*8)80,80,60
   60 L=N+1
      N=8*IJ+8
      DO 70 I=L,N
   70 B(I)=0.0
   80 GO TO(81,82),MM
   81 PUNCH 600
```

```
 82 K=0
    DO 95 I=1,N,8
    K=K+1
    GO TO(92,90),MM
 90 WRITE OUTPUT TAPE15,500,B(I),B(I+1),B(I+2),B(I+3),B(I+4),B(I+5),
   1B(I+6),B(I+7),K
    GO TO 95
 92 PUNCH 800,B(I),B(I+1),B(I+2),B(I+3),B(I+4),B(I+5),B(I+6),B(I+7)
 95 CONTINUE
    END FILE15
    REWIND15
    PRINT 400
    CALL EXIT
100 FORMAT(I9,E10.5)
200 FORMAT(3E10.5)
300 FORMAT(8E9.4,I4,3H SD)
400 FORMAT(58H    JOB FINISHED.  SAVE TPE A5 FOR OFF-LINE CARD PUNCHIN
   1G.////////////)
500 FORMAT(8F9.6,I4,2H P)
600 FORMAT(72X)
700 FORMAT(8E9.4)
800 FORMAT(8F9.6)
    END
```

Function ARCSIN(X)

```
    FUNCTION ARCSIN(X)
 10 A=+1.5707963
 20 B=-0.21459880
 30 C=+0.08897899
 40 D=-0.05017430
 50 E=+0.03089188
 60 F=-0.01708813
 70 G=+0.00667009
 80 H=-0.00126249
100 YY=X
110 IF(YY)   120,210,120
120 Y=ABSF(YY)
130 IF(Y-1.0)   140,230,280
140 Z=-SQRTF(1.0-Y)
150 Z=A+Z*(A+Y*(B+Y*(C+Y*(D+Y*(E+Y*(F+Y*(G+HY)))))))
160 IF(YY)   170,210,190
170 ARCSIN=  -Z
180 RETURN
190 ARCSIN=Z
200 RETURN
210 ARCSIN=0.0
220 RETURN
230 IF(YY)   260,210,240
240 ARCSIN=A
250 RETURN
260 ARCSIN=-A
270 RETURN
280 CALL ENDJOB
290  END
```

Subroutine RECIP

```
      SUBROUTINE RECIP(AR,BR,CR,ALR,BER,GAR,AA,BB,CC,COSAL,COSBE,COSGA)
      ALG=ALR*3.14159/180.0
      BEG=BER*3.14159/180.0
      GAG=GAR*3.14159/180.0
      COSAR=COSF(ALG)
      COSBR=COSF(BEG)
      COSGR=COSF(GAG)
      VR=AR*BR*CR*SQRTF(1.0-COSAR*COSAR-COSBR*COSBR-COSGR*COSGR+2.*COSAR
     1*COSBR*COSGR)
      SINAR=SINF(ALG)
      SINBR=SINF(BEG)
      SINGR=SINF(GAG)
      AA=BR*CR*SINAR/VR
      BB=AR*CR*SINBR/VR
      CC=AR*BR*SINGR/VR
      COSAL=(COSBR*COSGR-COSAR)/(SINBR*SINGR)
      COSBE=(COSAR*COSGR-COSBR)/(SINAR*SINGR)
      COSGA=(COSAR*COSBR-COSGR)/(SINAR*SINBR)
      RETURN
      END
```

Function DOTPROD

```
      FUNCTION DOTPRD(U,V,W,X,Y,Z,B1,B2,B3,COSA,COSB,COSC)
      DOTPRD=U*X*B1**2+V*Y*B2**2+W*Z*B3**2+(V*Z+Y*W)*B2*B3*COSA+
     1(U*Z+W*X)*B1*B3*COSB+(U*Y+V*X)*B1*B2*COSC
      RETURN
      END
```

Function SCAFAC

```
      FUNCTION SCAFAC(A,A1,B,B1,C,S)
      SCAFAC=A*EXPF(-A1*(S**2))+B*EXPF(-B1*(S**2))+C
      RETURN
      END
```

Subroutine MTXMUL

```
      SUBROUTINE MTXMUL(L,M,N,A,B,C)
      DIMENSION A(3,3),B(3,3),C(3,3)
      DO 10 I=1,L
      DO 10 J=1,N
   10 C(I,J)=0.
      DO 20 I=1,L
      DO 20 J=1,N
      DO 20 K=1,M
   20 C(I,J)=C(I,J)+A(I,K)*B(K,J)
      RETURN
      END
```

Function INTG(A)

```
      FUNCTION INTG(A)
      IF(A)20,10,20
   10 INTG=0
      GO TO 30
   20 INTG=XSIGNF(XINTF(ABSF(A)+.1),XINTF(A))
   30 RETURN
      END(2,2,2,2,2)
```

UNCLASSIFIED

Naval Research Laboratory. Report 5885.
A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS, by H.G. Norment. 71 pp., April 29, 1963.

This report contains descriptions and operating instructions for a collection of general utility programs applicable to various phases of crystal structure analysis with computers. All coding is done in FORTRAN II language for 32K core IBM 704 and 7090 machines; the FORTRAN-language programs are completely listed in the Appendix.

The data input to many of the programs has been designed to be compatible with the output of the

UNCLASSIFIED (over)

1. Mathematical computer programming
2. Crystal structure - Math. anal.
3. X-ray diffraction analysis - Data - Processing

I. FORTRAN

II. Norment, H. G.

UNCLASSIFIED

Naval Research Laboratory. Report 5885.
A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS, by H.G. Norment. 71 pp., April 29, 1963.

This report contains descriptions and operating instructions for a collection of general utility programs applicable to various phases of crystal structure analysis with computers. All coding is done in FORTRAN II language for 32K core IBM 704 and 7090 machines; the FORTRAN-language programs are completely listed in the Appendix.

The data input to many of the programs has been designed to be compatible with the output of the

UNCLASSIFIED (over)

1. Mathematical computer programming
2. Crystal structure - Math. anal.
3. X-ray diffraction analysis - Data - Processing

I. FORTRAN

II. Norment, H. G.

UNCLASSIFIED

Naval Research Laboratory. Report 5885.
A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS, by H.G. Norment. 71 pp., April 29, 1963.

This report contains descriptions and operating instructions for a collection of general utility programs applicable to various phases of crystal structure analysis with computers. All coding is done in FORTRAN II language for 32K core IBM 704 and 7090 machines; the FORTRAN-language programs are completely listed in the Appendix.

The data input to many of the programs has been designed to be compatible with the output of the

UNCLASSIFIED (over)

1. Mathematical computer programming
2. Crystal structure - Math. anal.
3. X-ray diffraction analysis - Data - Processing

I. FORTRAN

II. Norment, H. G.

UNCLASSIFIED

Naval Research Laboratory. Report 5885.
A COLLECTION OF FORTRAN PROGRAMS FOR CRYSTAL STRUCTURE ANALYSIS, by H.G. Norment. 71 pp., April 29, 1963.

This report contains descriptions and operating instructions for a collection of general utility programs applicable to various phases of crystal structure analysis with computers. All coding is done in FORTRAN II language for 32K core IBM 704 and 7090 machines; the FORTRAN-language programs are completely listed in the Appendix.

The data input to many of the programs has been designed to be compatible with the output of the

UNCLASSIFIED (over)

1. Mathematical computer programming
2. Crystal structure - Math. anal.
3. X-ray diffraction analysis - Data - Processing

I. FORTRAN

II. Norment, H. G.

automatic data reduction program XRDDR (H.G. Norment, "An X-Ray Diffraction Data Reduction Program for the IBM 704 and 7090," NRL Report 5739, Feb. 1962).

In the form presented in this report, the programs are written for use with the IBM 7090 IB Monitor system.

UNCLASSIFIED

UNCLASSIFIED

automatic data reduction program XRDDR (H.G. Norment, "An X-Ray Diffraction Data Reduction Program for the IBM 704 and 7090," NRL Report 5739, Feb. 1962).

In the form presented in this report, the programs are written for use with the IBM 7090 IB Monitor system.

UNCLASSIFIED

UNCLASSIFIED

automatic data reduction program XRDDR (H.G. Norment, "An X-Ray Diffraction Data Reduction Program for the IBM 704 and 7090," NRL Report 5739, Feb. 1962).

In the form presented in this report, the programs are written for use with the IBM 7090 IB Monitor system.

UNCLASSIFIED